Bound entanglement in $d \times d$ systems with symmetry

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Contents

1 Introduction

One calls a quantum system bipartite if it consists of two subsystems. Consider for example two atoms which have interacted with each other in the past but are now in two locally separated laboratories. If one cannot completely describe the states of the subsystems without the state of the whole quantum system the state is called *entangled*. Entanglement is the key resource that enables many quantum information processing tasks, and its detection and quantification has been considered at length in the past decades.

However, even in the bipartite case, open questions still remain to be answered. So-called bound entangled states are especially enigmatic, and remain elusive to be fully characterized both theoretically and experimentally. The definition of bound entangled states is that they cannot be used to generate a maximally entangled state under certain restrictions of the applicable operations in the experiment. Bound entanglement appears in highly mixed states, for which entanglement quantification methods are generically hard to implement. Mixed states are needed to describe experiments in which a specific (not mixed) quantum state can only be generated with a certain probability.

We introduce a family of highly symmetric, bipartite, mixed quantum states in arbitrary dimensions. It consists of all states that are invariant under local phase rotations and local cyclic permutations of the basis. We solve the separability problem for a subspace of these states and we show that a sizeable part of the family is bound entangled. We also calculate some of the Schmidt numbers for the family in $d = 3$. Schmidt numbers are quantifiers for the dimensionality of entanglement. Because our family is defined through symmetries, these results stand as a lower bound for the Schmidt number of generic non-symmetric states of the same dimension.

For dimension $d = 4$ we calculate a lower bound for the linear entropy which quantifies the amount of entanglement. Here we also carried out an extensive application of known methods to detect separability.

At the end we discuss some additional families of states. Those families are invariant under permutation of both subsystems. Here we mostly limit ourselves to describing the states and writing down the physicality constraints.

2 Mathematical Formulation of Quantum Theory

As a physical motivation for the postulates of quantum theory, we will briefly sketch the mathematical formulation of classical mechanics and address why it cannot describe quantum mechanics. In particular it will be shown that this abstract formulation of classical mechanics would not allow for Heisenberg's inequality. Since Isaac Newton's Principia Mathematica we know that it is often advantageous to model a classical system by treating position and momentum of a body as the state of the system. Then, the physical laws describe how one can calculate the second derivative of the position with respect to the time, the acceleration. In modern formulations of classical mechanics one wants to directly address the various restrictions on the space of all possible states. The movement of the body could for example be restricted by a rope. Likewise, in general relativity there is also a need for a general and sophisticated mathematical structure to describe the curvature of space-time. So in modern general formulations smooth manifolds are used to describe the set of all states. To be more precise, the cotangent space in a chart of the manifold gives us the coordinates for place and momentum of the particle or body. A physical quantity that can be determined by performing some measurement on the system is referred to as observable. Since in classical mechanics the state is completely determined if we know the position x and the momentum p, we can define our observables to be real functions in x and p. Because we see no reason why in this idealized model a determination of the state up to an arbitrarily small error should not allow an arbitrarily good determination of the quantity described by the observable, the observables are assumed to be continuous. For simplicity we also assume our manifold to be compact. A strong argument for this would be that every measurement device has a finite range. Now a definition for C^*-algebras will be given and we will notice that one can make use of this to describe observables.

Definition 2.1. A vector space (V,+) over the field $\mathbb{K} = \mathbb{R}$ or $= \mathbb{C}$ with the norm $||\cdot||$ and the product $\circ : V \times V \to V$ is a Banach algebra iff:

1. (V,+,$||\cdot||$) is a Banach space.
2. (V,+,$\circ$) is an associative $\mathbb{K}$-algebra.
3. $\forall A, B \in V \ ||A \circ B|| \leq ||A|| \cdot ||B||$

Definition 2.2. A C^*-algebra X is a Banach algebra over the field $\mathbb{C}$ with an endomorphism *. The map $\circ$ should have the following properties:

1. It is an involution: $\forall x \in X \quad x^{**} = (x^*)^* = x^*$
2. $\forall x, y \in X \quad (x + y)^* = x^* + y^*$
   $(xy)^* = y^* x^*$
3. $\forall x \in X$ and $\lambda \in \mathbb{C} \quad (\lambda x)^* = \overline{\lambda} x^*$
4. The C^*-identity is fulfilled: $\forall x \in X \quad ||x^* x|| = ||x^*||||x||$

Now we can equip the space of the observables (real continuous functions on manifold M) with a "+" and a "$\cdot$" operation, a norm, a scalar-multiplication and a conjugation, so that

Definition 2.3. For all $S \in M$ and $f, g \in \mathcal{C}_0(M, \mathbb{R})$

1. $(f+g)(S) = f(S) + g(S)$
2. $\forall a \in \mathbb{R} \quad (af)(S) = af(S)$
3. $(f \cdot g)(S) = f(S)g(S)$
4. $||f|| = \{|f(S)||S \in M\}$
5. $f^*(S) = \overline{f(S)}$

In [11] it is proven that, if we require this structure, one can describe the set of observables algebraic in the following way:

Theorem 2.1. The observables of a classical system are the self-adjoint elements of a separable commutative unital C^*-algebra $\mathcal{A}$.

Since we can describe the observables by making use of C^*-algebras the question arises, whether this is also possible for states.

Definition 2.4. Let a $\mathcal{A}$ be a C^*-algebra like in the definition 2.3. A map $S : \mathcal{A} \to \mathbb{C}, \quad f \mapsto f(S)$ is (also) called a state.

We can examine some properties of these classical states:

Theorem 2.2. For $S \in M$ the function $S : \mathcal{A} \to \mathbb{C}$ with $f \mapsto f(S)$ is a normalized linear positive functional.

Proof. $\forall f, g \in \mathcal{A},\ a \in \mathbb{R}$
Linearity: $S(f+ag) = (f+ag)(S) = f(S) + ag(S) = S(f) + aS(g)$
Positivity: $S(f \cdot g^*) = (f \cdot g^*)(S) = f(S)g^*(S) = f(S)\overline{g(S)} = S(f)\overline{S(g)}$
Normalisation: Let $\mathbf{1}$ be the observable $M \ni S \mapsto 1$. Now we get

$$||S|| = \sup_{||f||=1} f(S) \geq |S(\mathbf{1})| = 1.$$

On the other side we have

$$|S(f)| = |f(S)| \leq \sup_{S \in M} f(S) = ||f||$$
$$\Rightarrow ||S|| \leq 1$$

□

Now we will come to a contradiction of Heisenberg's uncertainty principle, which deems the presented formalism unsuited for describing quantum mechanics.
The Riesz-Markov theorem enables us to view the states as an average.

Theorem 2.3. For a locally compact Hausdorff space X, a state $S \in \mathcal{C}_0(X, \mathbb{R})$ can be written as

$$S(f) = \int_X f \mathrm{d}\mu_S.$$

In this integral representation μ_S is a uniquely determined probability measure.

Now $S(f)$ can be interpreted as an expectation value of the observable f, which is measured for the state S. This also justifies the following definition for the standard deviation.

Definition 2.5. For a state $S \in M$ and an observable $f \in \mathcal{C}_0(M, \mathbb{R})$ the variance is defined as

$$\sigma_S(f)^2 = S\left[(f - S(f))^2\right].$$

But for the definitions used in classical mechanics we introduced this yields

$$\sigma_S(f)^2 = S\left[(f - S(f))^2\right] = S\left[f^2 - 2S(f)f + S(f)^2\right] = f^2(S) - 2f(S)f(S) - (f(S))^2 = 0$$

This shows that to describe quantum mechanics we need a different mathematical formalism. To have no variance for all observables and states would contradict the famous Heisenberg uncertainty relation:

$$\sigma_S(p)\sigma_S(q) \geq \frac{1}{2}\hbar$$

Without further discussion we will now present the real mathematical framework for quantum mechanics as presented in [11].

Definition 2.6. The set of observables of a *quantum system* are exactly the self-adjoint elements of a separable (noncommunative) unital C^*-algebra $\mathcal{A}$.

Definition 2.7. The set of states $\mathcal{S}$ of a *quantum system* is the set of all positive linear functionals ψ on $\mathcal{A}$ so that $\psi(\mathbf{1}) = 1$.

The connection between this formulation of the mathematical framework of quantum mechanics and the axioms one learns in a usual quantum mechanics lecture [21], [5], [13] is given by the Gelfand-Naimark theorem.

Theorem 2.4. Gelfand-Naimark Theorem There exists a separable Hilbert space $\mathcal{H}$ over $\mathbb{C}$ so that

1. There exists an isometric *-isomorphism $\pi : \mathcal{A} \to \mathcal{H}$.
2. $\psi \in \mathcal{S}$, iff there exists a positive semi-definite, continuous, endomorphism $\Psi : \mathcal{H} \to \mathcal{H}$ (or $\Psi \in \mathcal{S}(\mathcal{H})$) , so that $\mathrm{Tr}(\Psi) = 1$ and for every $A \in \mathcal{A}$: $\psi(A) = \mathrm{Tr}(\Psi\pi(A))$.

A *-isomorphism is an isomorphism with the property $\pi(A^*) = \pi(A)^*$.
This thesis focuses mainly on quantum-mechanical systems, which can be divided into two smaller subsystems. In the next chapter we describe such a partition in detail, but the Gelfand-Naimark theorem already shows us, that we can study positive semi-definite self-adjoint operators over some Hilbert space to understand the states of the system.

2.1 Introduction to Bipartite Entanglement

In this thesis we will only consider bipartite systems. Physically, this means for example that two experimenters, Alice and Bob, each have one particle, which may have interacted with each other in the past. Furthermore we restrict ourselves to physical systems which can be described by a finite-dimensional Hilbert space. It suffices for this thesis to consider the complex Euclidean space $\mathbb{C}^d$. We use the bracket notation and thus denote an arbitrary orthonormal basis by:

$$|0\rangle := \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \quad |1\rangle := \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \ldots |d-1\rangle := \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}$$

We denote $|v\rangle \in \mathcal{H}$ as a vector in the Hilbert space $\mathcal{H}$ with $|| \, |v\rangle \, || = 1$. According to the Riesz representation theorem every element of the dual vector space can be written as the functional $\mathcal{H} \to \mathbb{C} \quad h \mapsto \langle v, h \rangle$, where v is a uniquely determined vector and the brackets denote the inner-product. This is the justification for the notation $\langle v|$ for an element of the dual vector space. If the decomposition of $|v\rangle$ in the standard basis is $|v\rangle = \sum_j v_j \, |j\rangle$ with $v_j \in \mathbb{C}$, the decomposition of $\langle v|$ is $\langle v| = \sum_j v_j^* \, \langle j|$. And with $\langle k| \, (|j\rangle) = \delta_{j,k}$, we see that $\langle w| \, (|v\rangle) = \langle w|v\rangle$ is just the Euclidean scalar product.

Until now we have not defined a mathematical structure to describe experiments, where some source produces quantum mechanical states only with certain probabilities. Consider for example an experiment where the states $|\psi_j\rangle \in \mathcal{H}$ for $j \in \{1, ..., n\}$ can be produced with the respective probabilities p_j and $\sum_j p_j = 1$. The correct mathematical framework for this sort of experiments is the set of positive semi-definite endomorphisms of $\mathcal{H}$. The situation in the example above is now described with linear maps of the form $\sum_j p_j P(|\psi_j\rangle)$, where $P(|\psi_j\rangle) =: |\psi_j\rangle \, \langle\psi_j|$ denotes the projector to the vector $|\psi_j\rangle$. We call the usual matrix representation of these endomorphisms density matrices. The condition that the classical probabilities should sum up to 1 and should not be negative leads to the requirement that density matrices have trace 1 and are positive semi-definite [16]. It should also be noted that for infinite dimensional systems, one has to define so called trace-class operators to ensure that the trace does not depend on the choice of the basis. If the state is already described by a vector in $\mathcal{H}$, we refer to it as pure state. The corresponding density matrix is in that case the projector to this vector. If a density matrix does not correspond to a pure state, we call the state it describes a mixed state.

To describe quantum-mechanical systems with multiple parties, the use of the tensor-product is advantageous. Let us consider again the situation where the experimenters Alice and Bob each have one particle. In addition we say that Alice can measure $d_A \in \mathbb{N}$ distinct values of, for example, energy at her particle. Similarly Bob can measure $d_B \in \mathbb{N}$ values. So all in all if both experimenters measure there are $d_A \cdot d_B$ different possible outcomes. The axioms of quantum mechanics suggest now that the whole state space

is given by $\mathbb{C}^{d_A \cdot d_B}$ (of course we actually have equivalence classes of unit vectors in $\mathbb{C}^{d_A \cdot d_B}$, where two elements are equivalent if they only differ by a complex phase). Since $\mathbb{C}^{d_A} \otimes \mathbb{C}^{d_B} \cong \mathbb{C}^{d_A \cdot d_B}$ the following notation is sensible:

$$\forall j \in \{1, ..., d_A\}, k \in \{1, ..., d_B\} \quad |j\rangle \otimes |k\rangle =: |j\rangle\,|k\rangle =: |j\ k\rangle\,.$$

Now the question arises whether and to what extent the experimental results of Alice and Bob are correlated. For a more precise description how these measurements are actually modelled in quantum theory we refer to [16]. To investigate such questions we need following definitions:

Definition 2.8. A quantum state $|\psi\rangle \in \mathbb{C}^{d_A} \otimes \mathbb{C}^{d_B}$ is called *separable*, if there exist $|\psi_A\rangle \in \mathbb{C}^{d_A}$ and $|\psi_B\rangle \in \mathbb{C}^{d_B}$ so that $|\psi\rangle = |\psi_A\rangle \otimes |\psi_B\rangle$. Otherwise we call the state $|\psi\rangle$ *entangled*.

For mixed states in $S(\mathcal{H}) := \{T \in \mathcal{L}(\mathcal{H}) | \operatorname{Tr}(T) = 1, T^\dagger = T, T \text{ is positive semi-definite}\}$, where $\mathcal{L}(\mathcal{H})$ denotes the continuous endomorphisms, we have a similar definition.

Definition 2.9. A state $\rho \in S(\mathbb{C}^{d_A} \otimes \mathbb{C}^{d_B})$ is called factorized or product state if there is $\rho_A \in \mathbb{C}^{d_A}$ and $\rho_B \in \mathbb{C}^{d_B}$ so that $\rho = \rho_A \otimes \rho_B$. If ρ is a convex combination of factorized states, we call it separable. Otherwise ρ is entangled.

The following theorem gives us an upper bound on the minimal number of summands in such convex combinations.

Theorem 2.5. Carathéodory:
Let $X \subseteq \mathbb{R}^n$. Then any point in a convex hull of X can be written as a convex combination of $n+1$ points of X.

Proof. see [3] □

We can consider $N \times N$-density matrices as a subset of Hermitian complex matrices with trace equal to 1. These matrices are described with $N-1+N(N-1)$ real parameters. Carathéodory's theorem therefore says that the convex sum can be written using only N^2 summands.
For bipartite pure states the problem of determining whether a state is entangled or not is quite manageable, as the following lemma shows:

Lemma 2.1. Schmidt decomposition:
Let $|\psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$ be a bipartite pure state. Then there exist two orthogonal bases $\{a_k | k \in \{1, ..., \dim(\mathcal{H}_1) =: d_A\}\}$ and $\{b_k | k \in \{1, ..., \dim(\mathcal{H}_2) =: d_B\}\}$ and real positive coefficients s_k, so that $|\psi\rangle = \sum_{k=1}^{\min\{d_A, d_B\}} s_k\,|a_k\rangle\,|b_k\rangle$.

Proof. First we expand $|\psi\rangle$ in some basis

$$|\psi\rangle = \sum_{k,j} \psi_{k,j}\,|k\rangle\,|j\rangle\,,$$

where $\psi_{k,j} := \langle j\ k|\psi\rangle$. Now we can do a singular value decomposition for the matrix $C := (\psi_{k,j})_{k,j}$. Thus there are two unitaries $U \in \mathbb{C}^{d_A \times d_A}$ and $V^\dagger \in \mathbb{C}^{d_B \times d_B}$ and a diagonal matrix $D \in \mathbb{R}^{d_A \times d_B}$, so that $C = UDV^\dagger$. The non-negative diagonal elements of D are called $D_{k,k} =: s_k$ for $k \in \{1, ..., \min\{d_A, d_B\}\}$. The following short calculation shows how the two basis have to be chosen:

$$\begin{aligned}
|\psi\rangle &= \sum_{k,j} \psi_{k,j} |k\rangle |j\rangle \\
&= \sum_{k,j} (UDV^\dagger)_{k,j} |k\rangle |j\rangle \\
&= \sum_{k,j} \sum_{l,m} U_{k,l} D_{lm} V^\dagger_{m,j} |k\rangle |j\rangle \\
&= \sum_l s_l \underbrace{\left(\sum_k U^T_{l,k} |k\rangle \right)}_{=:|a_l\rangle} \underbrace{\left(\sum_j V^\dagger_{l,j} |j\rangle \right)}_{=:|b_l\rangle}
\end{aligned}$$

□

The number of non-vanishing *Schmidt coefficients* (the s_k in the lemma above) is called Schmidt rank. In [26] the definition of Schmidt rank is extended to mixed states and called Schmidt number

Definition 2.10. For every pure state $|\psi\rangle$ in $\mathcal{H}_1 \otimes \mathcal{H}_2$ one can write the Schmidt rank r explicitly like $|\psi^r\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$. For $\rho \in S(\mathcal{H}_1 \otimes \mathcal{H}_2)$ the Schmidt number $K \in \mathbb{N}$ is given by

$$K := \min_{\{p_i \in [0,1],\quad |\psi_i^{r_i}\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2|\quad \rho = \sum_i p_i |\psi_i^{r_i}\rangle,\quad \sum_i p_i = 1\}} \max_i r_i.$$

If the Schmidt number is 1, there is a decomposition of ρ in separable states and ρ is separable. We denote the states that have a Schmidt number equal or less than K with S_K.

2.2 Separability criteria and completely positive maps

The separability problem is the task to determine, whether a given density matrix is separable or not. Since this problem is NP-hard [8] [15], one cannot expect to find a simple algorithm to solve it. The aim of this chapter is to introduce some more theory concerning this topic. The presented definitions and theorems can be found in section 6.3 of [16].

2.2.1 Entanglement Witnesses

Definition 2.11. A Hermitian operator $W \in \mathcal{L}(\mathcal{H}_A \otimes \mathcal{H}_B)$ is called entanglement witness, if for all factorized states $\psi \otimes \phi \in \mathcal{H}_A \otimes \mathcal{H}_B$, $\langle \psi \otimes \phi | W \psi \otimes \phi \rangle \geqslant 0$ and there exists at least one state $\eta \in \mathcal{H}_A \otimes \mathcal{H}_B$ with $\langle \eta | W \eta \rangle < 0$. If the scalar-product is negative for a particular state, we say that the witness detects the state (to be entangled).

Theorem 2.6. A state $\rho \in S(\mathcal{H}_A \otimes \mathcal{H}_B)$ is separable if and only if $\mathrm{tr}(\rho W) \geqslant 0$ for all entanglement witnesses W.

Proof. "⇒": Let ρ be a separable state. Then we can decompose it in product states, so that $\rho = \sum_j p_j \rho_A^j \otimes \rho_B^j$. We also can write the reduced density matrices as convex combinations of projectors, i.e. $\rho_A^j = \sum_k s_k^j \left|\psi_k^j\right\rangle \left\langle\psi_k^j\right|$ and $\rho_B^j = \sum_l t_l^j \left|\phi_l^j\right\rangle \left\langle\phi_l^j\right|$. Now one can directly calculate

$$\begin{aligned}\mathrm{tr}(\rho W) &= \sum_{j,k,l} p_j s_k^j t_l^j \,\mathrm{tr}\Big(\left|\psi_k^j\right\rangle \left\langle\psi_k^j\right| \otimes \left|\phi_l^j\right\rangle \left\langle\phi_l^j\right| W\Big) \\ &= \sum_{j,k,l} p_j s_k^j t_l^j \sum_{e,g} \left\langle e\middle|\psi_k^j\right\rangle \left\langle\psi_k^j\right| \otimes \left\langle g\middle|\phi_l^j\right\rangle \left\langle\phi_l^j\right| W \left|e\right\rangle \otimes \left|g\right\rangle .\end{aligned}$$

Using the relation $\sum_e |e\rangle \langle e|\psi\rangle = |\psi\rangle$ we get:

$$= \sum_{j,k,l} p_j s_k^j t_l^j \left\langle\psi_k^j\right| \otimes \left\langle\phi_l^j\right| W \left|\psi_k^j\right\rangle \otimes \left|\phi_l^j\right\rangle \geq 0.$$

"⇐": For the reverse direction we make use of theorem 3.4 in [19]. It states

Theorem 2.7. Let A and B be non-empty, disjoint, convex sets in a locally compact, real topological vector space X. If A is compact and B is closed then there exists a functional $\Lambda \in X^*$ and real numbers $r_1, r_2 \in \mathbb{R}$, so that for every $x \in A$ and $y \in B$

$$\Lambda(x) < r_1 < r_2 < \Lambda(y).$$

Here X^* denotes the dual vector space of X.

Consider the space $T(\mathcal{H}) := \{R \in \mathcal{L}(\mathcal{H}) | R \text{ is positive semi-definite}\}$ equipped with the trace norm $||R|| = (\mathrm{Tr}\Big(R^\dagger R\Big))^{\frac{1}{2}}$. For infinite dimensional systems one would also have to restrict to trace class operators, so that the trace is still well defined. Because this linear $\mathbb{R}$-vector space has a norm, it is also locally convex. Suppose ρ is an entangled state. We choose the set B to have ρ as its only element. For the set A we consider the separable states. This is a compact set in the tracenorm topology according to [16]. The dual space of the space $T(\mathcal{H})$ is the space $\mathcal{L}(\mathcal{H})$. From Theorem 2.7 and the representation theorem from Riesz it follows that there is a function $\Lambda \in \mathcal{L}(\mathcal{H})$, so that

$$\mathrm{tr}(\Lambda\eta) < r < \mathrm{tr}(\Lambda\rho)$$

for some $r \in \mathbb{R}$ and all $\eta \in T(\mathcal{H})$. Now $\Lambda - r\mathbb{I}$ is the desired entanglement witness. □

Positive maps are another mathematical construct that is helpful in deciding if a state is entangled.

Definition 2.12. We call Λ a linear map on $S(\mathcal{H})$ *positive*, if positive semi-definite elements of $S(\mathcal{H})$ are mapped to positive semi-definite elements.

To model a transformation between physical states, e.g. the state-transformation of a photon passing through a fiber, one needs an even stronger condition.

Definition 2.13. The linear mapping $\Lambda : \mathcal{L}(\mathcal{H}_A) \to \mathcal{L}(\mathcal{H}_A)$ is called *completely positive* iff for all finitely dimensional extensions $\mathcal{H}_B$ the mapping $\Lambda \otimes \mathbb{I}_B$ is positive on $\mathcal{L}(\mathcal{H}_A) \otimes \mathcal{L}(\mathcal{H}_B)$.

The following argument shows that these definitions are helpful in solving the separability problem. Consider two positive maps $\mathcal{F}_A \in \mathcal{L}(\mathcal{H}_A)$ and $\mathcal{F}_B \in \mathcal{L}(\mathcal{H}_B)$. With the tensor product we get the map $\mathcal{F} := \mathcal{F}_A \otimes \mathcal{F}_B \in \mathcal{L}(\mathcal{H}_A \otimes \mathcal{H}_B)$. Let ρ_{AB} be a separable state with the decomposition $\rho_{AB} = \sum_i p_i \rho_A^{(i)} \otimes \rho_B^{(i)}$. Now we apply the constructed map $\mathcal{F}_A \otimes \mathcal{F}_B$ to the state:

$$\mathcal{F}_A \otimes \mathcal{F}_B(\rho_{AB}) = \sum_i p_i \mathcal{F}_A(\rho_A^{(i)}) \otimes \mathcal{F}_B(\rho_B^{(i)})$$

Since the maps $\mathcal{F}_A$ and $\mathcal{F}_B$ are positive and the $\rho_A^{(i)}$ and $\rho_B^{(i)}$ are density matrices $\mathcal{F}_A(\rho_A^{(i)})$ and $\mathcal{F}_B(\rho_B^{(i)})$ are also positive semidefinite. Now it follows that $\mathcal{F}(\rho_{AB})$ is also positive semidefinite as sum of positive semidefinite operators. To detect some entangled states one makes use of the converse statement: If $\mathcal{F}(\rho)$ is not positive semidefinite, then ρ has to be entangled.

The following theorem provides further insight into the set of positive linear maps.

Theorem 2.8. Choi's theorem
For a positive linear map $\mathcal{E} : \mathcal{L}(\mathbb{C}_d) \to \mathcal{L}(\mathbb{C}_{d'})$ the following statements are equivalent:

1. $\mathcal{E}$ is completely positive.
2. $\mathcal{E} \otimes \mathrm{id}_d$ is a positive map.
3. The Choi matrix of $\mathcal{E}$ is positive.

The definition of the Choi matrix $\Phi_\mathcal{E}$ is that $(\Phi_\mathcal{E})_{mn} := \mathcal{E}(|\varphi_m\rangle \langle\varphi_n|)$, where the φ_j form an orthonormal basis of the Hilbert space $\mathbb{C}^d$.

Proof. 1.⇒ 2.: This follows immediately from the definition 2.13.
2.⇒ 3.: Consider the matrix $A = \sum_{m,n} |\varphi_m \otimes \varphi_m\rangle \langle\varphi_n \otimes \varphi_n|$. Since $A^\dagger = A$, $A^2 = dA$ and thus $A = \frac{1}{d} A A^\dagger$, this matrix is positive. Because $\mathcal{E} \otimes \mathrm{id}_d$ is positive we can apply it to A and still obtain a positive matrix. Applying the map yields $\mathcal{E} \otimes \mathrm{id}_d \sum_{m,n} |\varphi_m \otimes \varphi_m\rangle \langle\varphi_n \otimes \varphi_n| = \sum_{m,n} \mathcal{E}(|\varphi_m\rangle \langle\varphi_n|) \otimes |\varphi_m\rangle \langle\varphi_n| = \Phi_\mathcal{E}$ and thus the Choi matrix is positive.
3.⇒ 1.: Since $\Phi_\mathcal{E}$ is positive its eigenvalue decomposition has the following form:

$$\Phi_\mathcal{E} = \sum_{i=1}^{dd'} \lambda_i \tilde{\psi}_i \tilde{\psi}_i^\dagger,$$

where the $\tilde{\psi}_i$ are eigenvectors and $\lambda_i > 0$. One now defines $\psi_i = \frac{\tilde{\psi}}{\sqrt{\lambda_i}}$ and sees that

$$\Phi_{\mathcal{E}} = \sum_{i=1}^{dd'} \psi_i \psi_i^\dagger.$$

The tensor product $\mathbb{C}^{d'} \otimes \mathbb{C}^d$ can always be expressed as direct sum $\mathbb{C}^{d'} \otimes \mathbb{C}^d \simeq \mathbb{C}^{d'} \oplus ... \oplus \mathbb{C}^{d'}$. We define P_j as the projection to the jth such 'summand' in the direct sum of $\mathbb{C}^{d'}$ vector spaces. Now, the following equalities are valid

$$\mathcal{E}[|\phi_j\rangle \langle\phi_k|] = P_j \Phi_{\mathcal{E}} P_k = \sum_l P_j |\psi_l\rangle \langle\psi_l| P_k = \sum_l |P_j \psi_l\rangle \langle P_k \psi_l| . \tag{2.1}$$

Let for each $l \leq dd'$ the operator $V_l : \mathbb{C}^d \to \mathbb{C}^{d'}$ be defined by the equation

$$V_l \phi_j = P_j \psi_l.$$

Then equation 2.1 can be rewritten as:

$$\mathcal{E}[|\phi_j\rangle \langle\phi_k|] = \sum_l |P_j \psi_l\rangle \langle P_k \psi_l| = \sum_l |V_l \phi_j\rangle \langle V_l \phi_k| = \sum_l V_l |\phi_l\rangle \langle\phi_l| V_l^\dagger$$

Applying the linearity of $\mathcal{E}$ yields $\mathcal{E}(T) = \sum_l V_l T V_l^\dagger$ and it is well known that mappings of this form are completely positive.

□

With the help of Choi's theorem we are able to investigate the connection between positive maps and entanglement witnesses.

Theorem 2.9. Choi-Jamiolkowski isomorphism
Let $\mathcal{H}_d$ and $\mathcal{H}_{d'}$ be separable Hilbert spaces of dimensions d and d'. Furthermore φ_k is some orthonormal basis on $\mathcal{H}_d$. We define $P_+ := \frac{1}{d} \sum_{j,k=1}^{d} |\varphi_j \otimes \varphi_k\rangle \langle\varphi_j \otimes \varphi_k|$. The *Choi-Jamiolkowski isomorphism* is defined as follows

$$\begin{aligned} \mathcal{J} :& \{\mathcal{E} : \mathcal{L}(\mathcal{H}_d) \to \mathcal{L}(\mathcal{H}_{d'}) | \mathcal{E} \text{ is linear}\} \to \mathcal{L}(\mathcal{H}_d \otimes \mathcal{H}_{d'}) \\ & \mathcal{E} \mapsto \Omega_{\mathcal{E}} = \mathcal{E} \otimes \mathbb{I}[P_+] \end{aligned}$$

Proof. We will prove that the Choi-Jamiolkowski isomorphism is an injective homorphism. (As defined above the Choi-Jamiolkowski isomorphism is not surjective). The following mapping is inverse to $\mathcal{J}$:

$$\mathcal{J}^{-1} : \Omega \mapsto \mathcal{E}_\Omega : \mathcal{E}_\Omega[X] = d \operatorname{Tr}_2((\mathbb{I} \otimes X^T)\Omega)$$

The linearity of $\mathcal{J}$ and $\mathcal{J}^{-1}$ can be easily seen. That $\mathcal{J}^{-1}$ is inverse to $\mathcal{J}$ is shown by

following calculation:

$$\begin{aligned}
\forall X \in \mathcal{L}(\mathcal{H}_d) \quad \mathcal{J}^{-1}(\mathcal{J}(\mathcal{E}))[X] &= \mathcal{E}_{\Omega_\mathcal{E}}[X] \\
&= d\,\mathrm{Tr}_2((\mathbb{I}\otimes X^T)\Omega_\mathcal{E}) \\
&= d\,\mathrm{Tr}_2((\mathbb{I}\otimes X^T)\mathcal{E}\otimes\mathbb{I}[P_+]) \\
&= \sum_{j,k}\mathrm{Tr}_2((\mathbb{I}\otimes X^T)\mathcal{E}[|\varphi_j\rangle\langle\varphi_k|]\otimes|\varphi_j\rangle\langle\varphi_k|) \\
&= \sum_{j,k}\mathcal{E}[|\varphi_j\rangle\langle\varphi_k|]\,\mathrm{Tr}\Big(X^T|\varphi_j\rangle\langle\varphi_k|\Big) \\
&= \sum_{j,k}\mathcal{E}[|\varphi_j\rangle\langle\varphi_k|]\left\langle\varphi_k\middle|X^T\varphi_j\right\rangle \\
&= \mathcal{E}[\sum_{j,k}|\varphi_j\rangle\langle\varphi_k|\left\langle\varphi_k\middle|X^T\varphi_j\right\rangle] = \mathcal{E}[X]
\end{aligned}$$

Therefore we have that $\mathcal{J}^{-1}\circ\mathcal{J}$ is the identity operator and $\mathcal{J}$ is injective. □

Now we can formulate a proposition that relates the separability problem to positive maps:

Theorem 2.10. A state $\rho \in S(\mathcal{H}_A\otimes\mathcal{H}_B)$ is separable iff for all positive maps $\mathcal{F}: \mathcal{L}(\mathcal{H}_B)\to\mathcal{L}(\mathcal{H}_A)$ the operator $(\mathbb{I}\otimes\mathcal{F})(\rho)$ is positive.

Proof. Proof idea: We already know that the statement is true for linear entanglement witnesses. The Choi-Jamiolkowski isomorphism establishes a connection to positive maps. For an exact proof see [16]. □

2.2.2 PPT criterion

PPT is an abbreviation for positive partial transpose. The following lemma introduces one of the most important separability criteria.

Lemma 2.2. Let $\rho \in S(\mathcal{H}_A\otimes\mathcal{H}_B)$ a separable quantum state. Then the partial transpose of the ρ is positive semi-definite.

Proof. Since ρ is separable it can be decomposed into product states $\rho = \sum_k p_k\rho_k^A\otimes\rho_k^B$.

$$\rho^{T_B} = \left(\mathbb{I}\otimes(\cdot)^T\right)\rho = \sum_k p_k\rho_k^A\otimes(\rho_k^B)^T =: \tilde{\rho}$$

Since $(\rho_k^B)^T$ and thus $\tilde{\rho}$ are density matrices, they have to be positive semi-definite. □

2.2.3 CCNR criterion

Another important separability criterion is the Computable Cross Norm or Realignment (CCNR) criterion. The original papers, where it was introduced, are [20] and [4]. Before we present the criterion we have to define local orthogonal bases for matrices.

Definition 2.14. Consider a bipartite Hilbert space of the form $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$. We call $\{G_k^A \in \mathcal{L}(\mathcal{H}_A) | k \in \{1, ..., \dim(\mathcal{H}_A)\}\}$ a local orthogonal basis, if it is a basis of $\mathcal{L}_s(\mathcal{H})$ and the matrices are orthogonal with respect to the Hilbert-Schmidt scalar product, i.e.:

$$\forall k, j \in \{1, ..., n^2\} : \quad \mathrm{Tr}\Big(G_k^A G_j^A\Big) = \delta_{k,j}.$$

An example for a local orthogonal basis would be the generators of $SU(\dim(\mathcal{H}_A))$ normalized accordingly, together with the normalized identity matrix.

Theorem 2.11. The density matrix ρ can be decomposed as

$$\rho = \sum_k \lambda_k G_k^A \otimes G_k^B.$$

Then, if ρ is separable, $\sum_k \lambda_k \leq 1$.

Proof. The tensor product of the local orthogonal bases gives us a basis for Hermitian operators on $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$. Thus an arbitrary density matrix ρ can be decomposed as

$$\rho = \sum_{k,j} \mu_{k,j} G_k^A \otimes G_j^B.$$

Now one can perform a singular value decomposition for the matrix μ, so that we have unitary matrices U and V, as well as a diagonal matrix with entries λ_l and for all $l \neq 1 : \lambda_l = 0$. This yields

$$\begin{aligned}
\rho &= \sum_{k,j} (UDV^*)_{k,j} G_k^A \otimes G_j^B \\
&= \sum_{k,j,l} \lambda_l U_{k,l} (V^*)_{l,j} G_k^A \otimes G_j^B \\
&= \sum_l \lambda_l \left(\sum_k U_{k,l} G_k^A \right) \otimes \left(\sum_j (V^*)_{l,j} G_j^B \right) \\
&= \sum_l \lambda_l \tilde{G}_k^A \otimes \tilde{G}_j^B.
\end{aligned}$$

If ρ is a product state it is already of the form above with $\lambda_1 = 1$. On the set of density matrices one can define the Schatten-norms. The Schatten 1 norm is just the addition of all the singular values of the matrix. Now one can use the triangle inequality for the Schatten 1 norm of a separable state ρ

$$||\rho|| = || \sum_k p_k |a_k\rangle \langle a_k| \otimes |b_k\rangle \langle b_k| \, || \leq \sum_k p_k || \, |a_k\rangle \langle a_k| \otimes |b_k\rangle \langle b_k| \, || = 1$$

□

Another formulation of the CCNR criterion is given in [4] and [18]. The realigned matrix is related to the original density matrix as $R(\rho) = \sum_{i,j,k,l} \rho_{ij,kl} \, |ik\rangle \langle jl|$. It is known that $\mathrm{Tr} \sqrt{\rho^\dagger \rho} \leq 1$ for separable states.

2.3 Bound Entanglement

Assume that one can have arbitrary many copies of a quantum state ρ. If one is not able to produce a maximally entangled state ($|\phi\rangle = \sum_k \frac{1}{\sqrt{d}} |k\ k\rangle$) with this copies by using only local operations and classical communication, then ρ is called non-distillable. If ρ is also entangled, it is called bound entangled. The physical idea behind the phrase *local operations and classical communication* (LOCC) is the following. One can think of two experimenters at different places. They are allowed to communicate per classical means and tell each other what they measure. The system we are interested in can be thought of as two particles which may have interacted previously. Now each experimenter has one of these particles. The situation is depicted in figure 1.

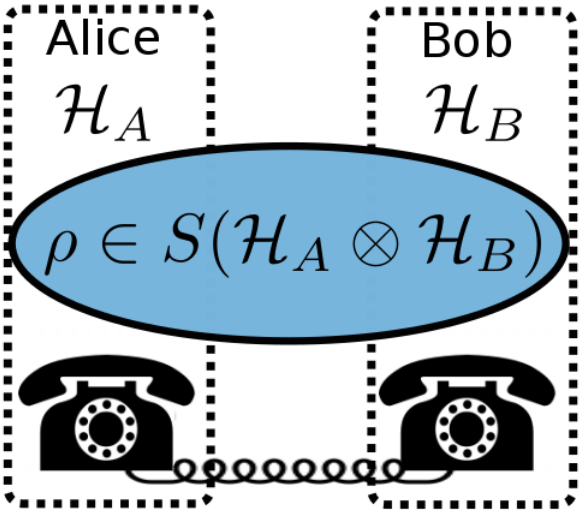

Figure 1: The experimenters, Alice and Bob, are locally separated, but able to communicate classically. Each one has only access two one of the two particles. The two particles together are in the quantum state ρ.

For a mathematical explication of LOCC we first have to define the notion of a channel. The physical time evolution can be described with a channel.

Definition 2.15. A *channel* $\mathcal{E}$ is a completely positive, linear map $\mathcal{E} : S(\mathcal{H}) \to S(\mathcal{H})$ that is trace nonincreasing.
We call a channel $\mathcal{E} : S(\mathcal{H}_A \otimes \mathcal{H}_B) \to S(\mathcal{H}_A \otimes \mathcal{H}_B)$ *local* if it can be written as $\mathcal{E} = \mathcal{E}_A \otimes \mathcal{E}_B$, where $\mathcal{E}_A$ and $\mathcal{E}_B$ are channels defined on $\mathcal{H}_A$ and $\mathcal{H}_B$, respectively.

Definition 2.16. A channel $\mathcal{E} : S(\mathcal{H}_A \otimes \mathcal{H}_B) \to S(\mathcal{H}_A \otimes \mathcal{H}_B)$ that is a sequence of local actions and exchange of classical communication is a *LOCC-channel*. Here an action is a channel or an instrument.

A quantum instrument is a mathematical model for a measurement. Although measurements in quantum mechanics are not a central topic for this thesis, we briefly mention the definition from [16].

Definition 2.17. Let (Ω, Σ) be a measurable space. A mapping $\mathcal{I} : \Sigma \to S(\mathcal{H})$ is called *instrument*, if it satisfies following properties:

1. For all $\rho \in S(\mathcal{H}) : \mathrm{Tr}(\mathcal{I}(\Omega)[\rho]) = 1 \quad \mathrm{Tr}(\mathcal{I}(\emptyset)[\rho]) = 0$
2. For all $\rho \in S(\mathcal{H}$ and all sequences of mutually disjoint sets $\{X_j\}$, with $X_j \in \Sigma$, $\mathcal{I}$ has to fulfil
$$\mathrm{Tr}(\mathcal{I}(\cup_j X_j)[\rho]) = \sum_j \mathrm{Tr}(\mathcal{I}(X_j)[\rho])$$

The exchange of classical information can be used in the following way. Suppose one wants to implement a convex sum of factorized channels i.e. $\mathcal{E} = \sum_j q_j \mathcal{E}_j^A \otimes \mathcal{E}_j^B$. Now the $(q_1, q_2..)$ can be interpreted as probability distribution. The idea for the implementation is that Alice generates the index-number j according to the probability distribution q_j. Then she tells Bob the number that she generated. If Alice generated the number $k \in \mathbb{N}$ they know that they have to implement $\mathcal{E}_k^A \otimes \mathcal{E}_k^B$.

LOCC protocols can have a quite involved structure, since the measurements one party performs can depend on the measurement outcomes of the other party. To illustrate this we have a look at a LOCC communication protocol consisting of n communication rounds (s. Def. 6.16 in [16]). Bob starts by performing a measurement, which can be described with the instrument $\Omega_1 \ni j \to \mathcal{F}_j^B$, where $\mathcal{F}_j^B$ are operations and Ω_1 is an outcome space. From definition 2.17 1. and 2. we know that the sum $\sum_{j_1 \in \Omega_1} \mathcal{F}_{j_1}^B =: \mathcal{E}_1^B$ is trace preserving for density matrices. Now Bob can communicate the result of the measurement $j_1 \in \Omega_1$ to Alice. In the second round she does a measurement with the outcome space Ω_2 and the operations $\mathcal{F}_{j_2}^A$. Alice can then also communicate her results to Bob and they continue with procedures of this sort. At the end they both can implement a local channel $\mathcal{E}_{n+1|j_n...j_1}^A \otimes \mathcal{E}_{n+1|j_n...j_1}^B$. This notation should emphasize that this last channel depends on the previously exchanged information about the measurements $j_1...j_n$. The final channel for this LOCC protocol is:

$$\mathcal{E}_{LOCC} = \sum_{j_n,...,j_2,j_1} (\mathcal{E}_{n+1|j_n,...,j_1}^A \otimes \mathcal{E}_{n+1|j_n,...,j_1}^B)...(\mathcal{F}_{j_2|j_1}^A \otimes \mathcal{F}_{j_1}^B)),$$

where $\sum_{j_2} \mathcal{F}_{j_2|j_1}^A = \mathcal{E}_{2|j_1}^A$ etc. and $\mathcal{E}_{n+1|j_n,...,j_1}^A$, $\mathcal{E}_{n+1|j_n,...,j_1}^B$ are channels. In figure 2 there is a sketch of the described LOCC protocol.

In [1] there is a characterisation of distillability that does not use LOCC protocols anymore.

Definition 2.18. Let $\rho \in S(\mathcal{H}_A \otimes \mathcal{H}_B)$ be a bipartite quantum state. If for $n \in \mathbb{N}$ there exist two-dimensional projectors P and Q, such that $\left(P \otimes Q\ \rho^{\otimes n}\ (P \otimes Q)^T\right)^{T_A}$ has at least one negative eigenvalue, then ρ is called *n-distillable*.

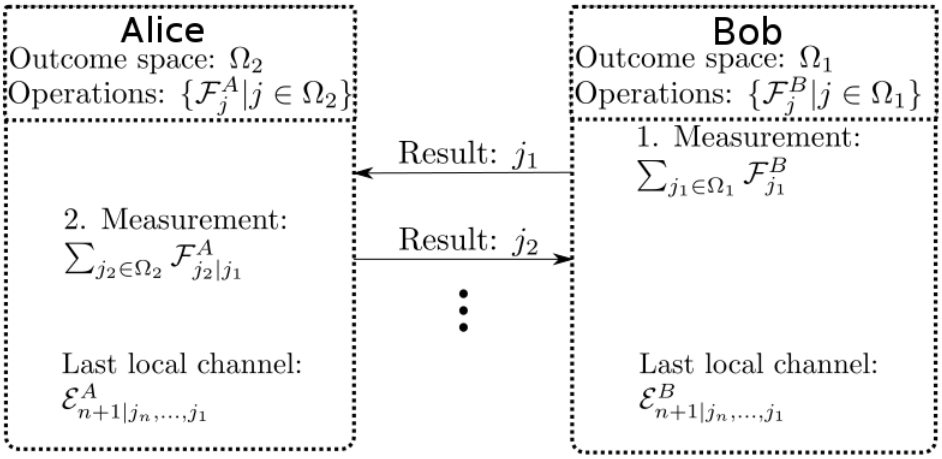

Figure 2: Schematic of an LOCC communication protocol consisting of n communication rounds.

A state is not distillable, if and only if it is not n-distillable for all $n \in \mathbb{N}$. It was already proven in [17] that the PPT condition implies the non distillable property. Whether the converse is also true, is a famous open problem in quantum information. Therefore it is not known yet if there is a bound entangled state with a partial transpose that has at least one negative eigenvalue (NPT).

3 Convex roof of entanglement monotones

A frequent question in quantum information theory is how strong the entanglement between particles in a certain state is [14]. Such entanglement quantification is important, because one often thinks of entanglement as a kind of useful resource for certain tasks in quantum computation. To know how entangled a given state is we define entanglement measures.

Definition 3.1. If a function $E : S(\mathcal{H}) \longrightarrow \mathbb{R}^+ \cup 0$ fulfils the following conditions, it is called entanglement measure or entanglement monotone.

1. All separable states are mapped to zero.

2. If we change the basis locally on all sites the amount of entanglement stays the same. Therefore for every unitary U we want to have $E(\rho) = E(U \otimes U\rho U^\dagger \otimes U^\dagger)$.

3. In experiments one cannot increase the amount of entanglement by simply performing local operations, even if all the experimenters can use classical communication. If the positive map Λ corresponds to an LOCC protocol, we therefore have:

$$E(\rho) \geq E(\Lambda(\rho))$$

4. E is convex:
$$E(\sum_k p_k \rho_k) \leq \sum_k p_k E(\rho_k)$$

5. E is additive: $E(\rho^{\otimes n}) = nE(\rho)$. An even stronger condition is $E(\rho_A \otimes \rho_B) = E(\rho_A) + E(\rho_B)$.

It should be noted that this is not the only possible definition of an entanglement monotone. Indeed some functions which are not convex are still called entanglement monotones. Furthermore, the fifth property is often difficult to prove.

A popular entanglement monotone is the entanglement of formation. It can be constructed as follows

Definition 3.2. Let $|\psi\rangle$ be a pure quantum state. The entanglement of formation is given via the Von Neumann entropy

$$E(|\psi\rangle\langle\psi|) = -\operatorname{Tr}\left(\rho_A \log(\rho_A)\right),$$

where

$$\rho_A = \operatorname{Tr}_B(|\psi\rangle\langle\psi|) = \operatorname{Tr}_B(\sum_{k,l,m,n} \psi_{k,l,m,n} |kl\rangle\langle mn|) = \sum_{k,l,m} \psi_{k,l,m,l} |k\rangle\langle m|$$

is the marginal state of Alice and $\operatorname{Tr}_B(\cdot)$ is the partial trace operation.

If we have an entanglement monotone that is defined on the pure states we can extend it to mixed states with the so called *convex roof extension*.

Definition 3.3. If E denotes an entanglement monotone on the pure states the convex-roof extension $\hat{E} : S(\mathcal{H}_A \otimes \mathcal{H}_B) \to \mathbb{R}_+ \cup 0$ is given by

$$\hat{E}(\rho) = \inf_{\{p_k \in [0,1],\ |\psi_k\rangle|\ \rho = \sum_k p_k |\psi_k\rangle\langle\psi_k|,\ \sum_k p_k = 1\}} \sum_k p_k E(|\psi_k\rangle\langle\psi_k|)$$

The convex roof extension of the Von Neumann entropy is called the entanglement of formation. The formula for the Shannon entropy can of course be expanded as a Taylor series around $(x = 1)$

$$-x\log(x) = -[(x-1) + \frac{1}{2}(x-1)^2 + ...] = \frac{1}{2} - \frac{x^2}{2}...$$

This formula is also meaningful if we insert ρ for x and write $\rho = \mathbb{I}$ instead of $x = 1$. One would in particular define the logarithm of a bounded, linear operator as the power series in functional calculus. This motivates the following formula for the linear entropy E_{lin}.

$$E_{\text{lin}}(|\psi\rangle) = 1 - \operatorname{Tr}\Big(\rho_A^2\Big). \tag{3.1}$$

The second term $\operatorname{Tr}(\rho_A^2)$ is called purity of $\rho_A = \operatorname{Tr}_B(|\psi\rangle\langle\psi|)$. We want to prove that it fulfils some of the properties of an entanglement monotone. For this purpose we investigate some well-known properties of the purity, which are described in proposition 2.13 from [16].

Proposition 3.1. The purity $\mathcal{P}(\rho) := \mathrm{Tr}(\rho^2)$ fulfils the properties

1. Convexity:

$$\forall \rho_1, \rho_2 \in S(\mathcal{H}), \lambda \in [0,1] \quad \mathcal{P}(\lambda\rho_1 + (1-\lambda)\rho_2) \leq \lambda\mathcal{P}(\rho_1) + (1-\lambda)\mathcal{P}(\rho_2)$$

2. Invariance under unitary conjugation:

$$\forall U \in U(\mathcal{H}) \quad \mathcal{P}(U\rho U^\dagger) = \mathcal{P}(\rho)$$

3. $\mathcal{P}(\rho) = 1 \quad \Leftrightarrow \quad \rho$ is pure

Proof. **1.:** The left side of the inequality is

$$\mathcal{P}(\lambda\rho_1 + (1-\lambda)\rho_2) = \mathrm{Tr}\Big(\lambda^2\rho_1^2 + \lambda(1-\lambda)(\rho_1\rho_2 + \rho_2\rho_1) + (1-\lambda)^2\rho_2^2\Big).$$

On the right side we have

$$\lambda\mathcal{P}(\rho_1) + (1-\lambda)\mathcal{P}(\rho_2) = \lambda\,\mathrm{Tr}\Big(\rho_1^2\Big) + (1-\lambda)\,\mathrm{Tr}\Big(\rho_2^2\Big)$$

By subtracting the right side from the left one, we get the difference Δ:

$$\begin{aligned}\Delta &= (\lambda - \lambda^2)\,\mathrm{Tr}\Big(\rho_1^2\Big) + ((1-\lambda) - (1-\lambda)^2)\,\mathrm{Tr}\Big(\rho_2^2\Big) - \lambda(1-\lambda)\,\mathrm{Tr}(\rho_1\rho_2 + \rho_2\rho_1) \\ &= \lambda(1-\lambda)\,\mathrm{Tr}\Big(\rho_1^2 + \rho_2^2 - \rho_1\rho_2 - \rho_2\rho_1\Big) \\ &= \lambda(1-\lambda)\,\mathrm{Tr}\Big((\rho_1+\rho_2)^2\Big)\end{aligned}$$

This is always greater than zero, because $\lambda(1-\lambda)$ and $\mathrm{Tr}((\rho_1+\rho_2)^2)$ are positive. $(\rho_1+\rho_2)^2$ is positive semi-definite as sum and product of positive semi-definite matrices. And since the trace is just the sum of all eigenvalues the term $\mathrm{Tr}((\rho_1+\rho_2)^2)$ is greater than zero.
2.: Since U is unitary we can use $U^\dagger U = \mathbb{I}$ and $\sum_k U^\dagger)_{m,k} U_{k,l} = \delta_{m,l}$.

$$\begin{aligned}\mathcal{P}(U\rho U^\dagger) &= \mathrm{Tr}\Big(U\rho U^\dagger U\rho U^\dagger\Big) = \mathrm{Tr}\Big(U\rho^2 U^\dagger\Big) \\ &= \sum_k \langle k|\, U\rho^2 U^\dagger\, |k\rangle = \sum_{k,l,m} U_{k,l}(\rho^2)_{l,m}(U^\dagger)_{m,k} = \sum_{l,m}(\rho^2)_{l,m}\delta_{l,m} \\ &= \mathrm{Tr}\Big(\rho^2\Big) = \mathcal{P}(\rho)\end{aligned}$$

3.: " $\Leftarrow$:" For $|\phi\rangle \in \mathcal{H}$ we get:

$$\mathrm{Tr}\Big((|\phi\rangle\langle\phi|)^2\Big) = \mathrm{Tr}(|\phi\rangle\langle\phi|) = 1$$

For a clarification of the equivalence of pure states and one dimensional projections and a proof of 3. see Proposition 2.11 in [16].
"$\Rightarrow$:" We proof this by contraposition. Since $\rho \in S(\mathcal{H})$ is a mixed state, we can write it

as $\rho = \lambda\rho_1 + (1-\lambda)\rho_2$ for some $\lambda \in \mathbb{R}$ and $\rho_1, \rho_2 \in S(\mathcal{H})$ with $\rho_1 \neq \rho_2$. The purity for this state can be bounded using the Cauchy Schwartz inequality on $|\mathrm{Tr}(\rho_1\rho_2)|$.

$$\begin{aligned}\mathcal{P}(\lambda\rho_1 + (1-\lambda)\rho_2) &= \mathrm{Tr}\Big(\lambda^2\rho_1^2 + \lambda(1-\lambda)(\rho_1\rho_2 + \rho_2\rho_1) + (1-\lambda)^2\rho_2^2\Big) \\ &\leq \lambda^2\,\mathrm{Tr}\Big(\rho_1^2\Big) + 2\lambda(1-\lambda)\sqrt{\mathrm{Tr}(\rho_1^2)\,\mathrm{Tr}(\rho_2^2)} + (1-\lambda)^2\,\mathrm{Tr}\Big(\rho_2^2\Big) \\ &\leq \lambda^2 + 2\lambda(1-\lambda) + (1-\lambda)^2 = 1\end{aligned}$$

In the last step we used that for all $\rho \in S(\mathcal{H})$ $\mathrm{Tr}(\rho^2) \leq 1$, which is proven after definition 2.10 in [16]. Since we assumed $\rho_1 \neq \rho_2$ and those two states are not linear dependent, so that the Cauchy Schwartz inequality cannot be tight. $\mathcal{P}(\rho) < 1$ follows from this. □

We want to prove that property 1 in Definition 3.1 is fulfilled for the linear entropy. A pure separable state $|\psi\rangle$ is just a product state $|\psi\rangle = |\psi_A\rangle \otimes |\psi_B\rangle$. Now since $\mathrm{Tr}_A(|\psi\rangle\langle\psi|) = |\psi_B\rangle\langle\psi_B|$ is a pure state, the purity is 1 and the linear entropy is zero. For mixed states there is a decomposition in separable pure states. So the infimum of the convex roof extension is here obtained at zero.
The second condition in definition 3.1 follows directly from Proposition 3.1 part 2, since local unitaries are unitary.

The convexity of the linear entropy arises because of the convex roof extension. From part 1 of Proposition 3.1 one would think that the linear entropy is concave. But if one has the two distinct pure states ρ_1 and ρ_2, their mixture $\lambda\rho_1 + (1-\lambda)\rho_2$ is a mixed state. Therefore we have:

$$\begin{aligned}\hat{E}(\lambda\rho_1 + (1-\lambda)\rho_2) &= \inf_{\{p_k\in[0,1],\,|\psi_k\rangle|\quad \rho=\sum_k p_k|\psi_k\rangle\langle\psi_k|,\ \sum_k p_k=1\}} \sum_k p_k E(|\psi_k\rangle\langle\psi_k|) \\ &\leq \lambda E(\rho_1) + (1-\lambda)E(\rho_2) = \lambda\hat{E}(\rho_1) + (1-\lambda)\hat{E}(\rho_2)\end{aligned}$$

In [28] there is an extensive proof how the convex roof extension works. It can be applied to the linear entropy of pure states because of the properties presented in Proposition 3.1.

For a pure state $|\psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$ the linear entropy satisfies

$$E_{\mathrm{lin}} = \sum_{jklm} |\psi_{jk}\psi_{lm} - \psi_{jm}\psi_{lk}|^2, \tag{3.2}$$

where $\psi_{jk} := \langle j\ k|\psi\rangle$. The proof of this identity will be given at the end of section 4.1.4.

3.1 Families of symmetric states

In the bipartite case the dimension of the Hilbert-space of the whole system scales with d^2, if the dimension of the sub-system is d. Therefore it may not always be possible to prove statements for the whole state space. To nevertheless get some results for high

sub-system dimensions d, one can focus on small symmetric families of states. The families of states F that we investigate in this thesis are symmetric under certain local unitaries $\mathrm{Sym} \subset U(\mathcal{H})$ in the sense that

$$\rho \in F \subset S(\mathcal{H}) \Leftrightarrow (U \otimes U^*)\rho(U \otimes U^*)^\dagger = \rho \quad \forall U \in \mathrm{Sym}. \tag{3.3}$$

We consider the following set of local unitaries:

$$\mathcal{G} := \{U \otimes U^* | U \in \mathrm{Sym}\}$$

A motivation why we are mainly considering local unitaries of the above form is that the maximal entangled state $|\phi\rangle = \frac{1}{\sqrt{d}} \sum_{j=0}^{d-1} |j\rangle \otimes |j\rangle$ is invariant under them. If we insert the density matrix of the maximally entangled state for ρ we get

$$\begin{aligned}
&\frac{1}{d}(U \otimes U^*) \sum_{j,k} |jj\rangle \langle kk| (U \otimes U^*)^\dagger \\
&= \frac{1}{d} \sum_{j,k} U |j\rangle \langle k| U^\dagger \otimes U^* |j\rangle \langle k| (U^*)^\dagger.
\end{aligned}$$

One sees that this is just some basis change. The state above can again be written as a vector in $\mathcal{H} \otimes \mathcal{H}$

$$\begin{aligned}
&U \otimes U^* \frac{1}{\sqrt{d}} \sum_{j=0}^{d-1} |j\rangle \otimes |j\rangle \\
&= \frac{1}{\sqrt{d}} \sum_{j=0}^{d-1} \sum_k U_{k,j} |k\rangle \otimes \sum_l U^*_{l,j} |l\rangle \\
&= \frac{1}{\sqrt{d}} \sum_k \sum_l \sum_{j=0}^{d-1} U_{k,j} \cdot U^*_{l,j} |k\rangle \otimes |l\rangle \\
&= \frac{1}{\sqrt{d}} \sum_k \sum_l \delta_{k,l} |k\rangle \otimes |l\rangle \\
&= \frac{1}{\sqrt{d}} \sum_k |k\rangle \otimes |k\rangle \\
&= |\phi\rangle .
\end{aligned}$$

We first want to look at the case where the unitaries $U \in \mathrm{Sym}$ are of the form

$$U = e^{i \sum_j \varphi_j \mathfrak{g}_j},$$

where the $\mathfrak{g}_j$ are diagonal generators of SU(d) and $\varphi_j \in \mathbb{R}$. One possible representation of the diagonal generators is

$$\mathfrak{g}_j = \frac{1}{\sqrt{j(j+1)}} \begin{pmatrix} 1 & 0 & & & & & & & \\ 0 & 1 & & & & & & & \\ & & \ddots & & & & & & \\ & & & 1 & & & & & \\ & & & & -j & & & & \\ & & & & & 0 & & & \\ & & & & & & \ddots & & \\ & & & & & & & 0 & 0 \\ & & & & & & & 0 & 0 \end{pmatrix}$$

Here the matrix element $-j$ is in the j-th position. It is obvious that, by choosing the phases φ_j properly, every real diagonal traceless matrix $A =: \mathrm{diag}(\theta_1, \ldots, \theta_d)$ can be written as $\sum_j \varphi_j \mathfrak{g}_j$. The corresponding element in SU(d) is

$$U = \begin{pmatrix} e^{i\theta_1} & 0 & & \\ 0 & e^{i\theta_2} & & \\ & & \ddots & \\ & & & e^{i\theta_d} \end{pmatrix}.$$

And we not only know from basic theory about Lie-algebras [22], but also see directly that:

$$\det(U) = e^{i\sum_j \theta_j} = e^{i0} = 1$$

Now we evaluate equation 3.3 for this group of unitaries

$$\begin{aligned} &\forall \theta_1, ..., \theta_d \in \mathbb{R} \ (\sum_j e^{i\theta_j} |j\rangle \langle j| \otimes \sum_j e^{-i\theta_j} |j\rangle \langle j|) \rho (\sum_j e^{-i\theta_j} |j\rangle \langle j| \otimes \sum_j e^{i\theta_j} |j\rangle \langle j|) = \rho \\ &\Leftrightarrow \forall \theta_1, ..., \theta_d \in \mathbb{R} \ \sum_j \sum_k \sum_l \sum_m e^{i(\theta_j - \theta_k - \theta_l + \theta_m)} |jk\rangle \langle jk| \left(\rho_{jk,lm} |jk\rangle \langle lm|\right) |lm\rangle \langle lm| = \rho \\ &\Leftrightarrow \forall \theta_1, ..., \theta_d \in \mathbb{R} \ \forall j,k,l,m \in \{1, ..., d\} \quad e^{i(\theta_j - \theta_k - \theta_l + \theta_m)} \rho_{jk,lm} = \rho_{jk,lm} \\ &\Leftrightarrow \rho_{jk,lm} = 0 \text{ for } (j \neq k \vee l \neq m) \wedge (j \neq l \vee k \neq m) \end{aligned}$$

Another requirement for density matrices is that they fulfil $\mathrm{tr}(\rho) = \sum_{j,k} \rho_{jk,jk} = 1$. They also have to be Hermitian. Therefore we get for the parameters $\forall j,k \in \{1, ..., d\}$: $\rho_{jj,kk} = \rho^*_{kk,jj}$. Since ρ also needs to be positive semi-definite, one knows already that $\forall j,k \in \{1, ..., d\}, \quad j \neq k, \quad \rho_{jk,jk} \geq 0$. Together with this last condition it would suffice to know that $(A)_{j,k} := \rho_{jj,kk}$ is positive semi-definite to deduce that ρ is positive semi-definite. If we do not restrict ourselves to a smaller family we of course cannot expect to get simple formulas for the coefficients that tell us if the matrix is a density matrix and corresponds to a state.

Next we want to investigate the PPT condition, e.g., for which parameters is the partial transposed density matrix positive semi-definite. We will show the computation for $d = 3$ and notice that the calculation can be generalized. The density matrix has the form:

$$\begin{pmatrix}
\rho_{00,00} & 0 & 0 & 0 & (\rho_{11,00})^* & 0 & 0 & 0 & (\rho_{22,00})^* \\
0 & \rho_{01,01} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \rho_{02,02} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \rho_{10,10} & 0 & 0 & 0 & 0 & 0 \\
\rho_{11,00} & 0 & 0 & 0 & \rho_{11,11} & 0 & 0 & 0 & (\rho_{22,11})^* \\
0 & 0 & 0 & 0 & 0 & \rho_{12,12} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \rho_{20,20} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \rho_{21,21} & 0 \\
\rho_{22,00} & 0 & 0 & 0 & \rho_{22,11} & 0 & 0 & 0 & \rho_{22,22}
\end{pmatrix}.$$

Applying the partial transpose yields:

$$\begin{pmatrix}
\rho_{00,00} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \rho_{01,01} & 0 & (\rho_{11,00})^* & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \rho_{02,02} & 0 & 0 & 0 & (\rho_{22,00})^* & 0 & 0 \\
0 & \rho_{11,00} & 0 & \rho_{10,10} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \rho_{11,11} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \rho_{12,12} & 0 & (\rho_{22,11})^* & 0 \\
0 & 0 & \rho_{22,00} & 0 & 0 & 0 & \rho_{20,20} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \rho_{22,11} & 0 & \rho_{21,21} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \rho_{22,22}
\end{pmatrix}.$$

To investigate when the matrix is positive semi-definite we reorder the basis and get the matrix:

$$\begin{pmatrix}
\rho_{01,01} & (\rho_{11,00})^* & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\rho_{11,00} & \rho_{10,10} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \rho_{02,02} & (\rho_{22,00})^* & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \rho_{22,00} & \rho_{20,20} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \rho_{12,12} & (\rho_{22,11})^* & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \rho_{22,11} & \rho_{21,21} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \rho_{00,00} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \rho_{11,11} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \rho_{22,22}
\end{pmatrix}.$$

This is clearly a block diagonal matrix. Therefore it is positive semi-definite if the blocks are positive semi-definite. Since at the upper left corner there are just 2×2 blocks one has to calculate the determinant of those. This caluculation can be generalized to higher dimension. To be PPT a state ρ in our family has to fulfil $\rho_{kk,kk} \geq 0$ and

$$\forall k,j \in \{0,...,d-1\}, k>j: \ \det\begin{pmatrix} \rho_{jk,jk} & \rho^*_{kk,jj} \\ \rho_{kk,jj} & \rho_{kj,kj} \end{pmatrix} \geq 0 \tag{3.4}$$

$$\Rightarrow \rho_{jk,jk}\rho_{kj,kj} \geq |\rho_{kk,jj}|^2.$$

The family is still quite general and, as it is, it is hard to compute e.g. the CCNR condition explicitly. To illustrate this we show the realigned matrix for dimension $d = 3$. It is

$$\begin{pmatrix}
\rho_{0,0,0,0} & 0 & 0 & 0 & \rho_{0,1,0,1} & 0 & 0 & 0 & \rho_{0,2,0,2} \\
0 & (\rho_{1,1,0,0})^* & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & (\rho_{2,2,0,0})^* & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \rho_{1,1,0,0} & 0 & 0 & 0 & 0 & 0 \\
\rho_{1,0,1,0} & 0 & 0 & 0 & \rho_{1,1,1,1} & 0 & 0 & 0 & \rho_{1,2,1,2} \\
0 & 0 & 0 & 0 & 0 & (\rho_{2,2,1,1})^* & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \rho_{2,2,0,0} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \rho_{2,2,1,1} & 0 \\
\rho_{2,0,2,0} & 0 & 0 & 0 & \rho_{2,1,2,1} & 0 & 0 & 0 & \rho_{2,2,2,2}
\end{pmatrix}.$$

Reordering the basis yields:

$$\begin{pmatrix}
\rho_{0,0,0,0} & \rho_{0,1,0,1} & \rho_{0,2,0,2} & 0 & 0 & 0 & 0 & 0 & 0 \\
\rho_{1,0,1,0} & \rho_{1,1,1,1} & \rho_{1,2,1,2} & 0 & 0 & 0 & 0 & 0 & 0 \\
\rho_{2,0,2,0} & \rho_{2,1,2,1} & \rho_{2,2,2,2} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & (\rho_{1,1,0,0})^* & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & (\rho_{2,2,0,0})^* & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \rho_{1,1,0,0} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & (\rho_{2,2,1,1})^* & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \rho_{2,2,0,0} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \rho_{2,2,1,1}
\end{pmatrix}.$$

Now there is a real matrix in the upper left corner that is quite general and does not have many properties. If we knew that it is diagonalizable we had some simple way to estimate the sum of the singular values. In the last chapter we investigate the case, where we have symmetry under permutation of both subsystems, so that $\rho_{ij,kl} = \rho_{ji,lk}$. In this case the upper left matrix is symmetric and thus diagonalisable with real eigenvalues.

One can add other unitaries to the set Sym to further reduce the number of parameters. A reasonable demand is that Sym is still a group afterwards. To this end we add to Sym a group of basis-element-permutations, which is a subgroup G of the symmetric group $S(d)$. Because of the invariance under local phase rotations, the positions of all non-vanishing basis elements only depend on two local basis elements (at least two of the four indices are always the same). In terms of algebra, we are interested in the orbit of the diagonal subgroup of $G \times G$. Matrix elements that are both elements of the same

orbit then have the same parameter. For the non-diagonal elements of ρ one also has to keep in mind that ρ is symmetric.

3.2 Convex characteristic curve method

The convex roof of entanglement monotones is very hard to compute for an arbitrary state. However, for families of symmetric states a method is presented in [23], to calculate such entanglement monotones. The method is described by following theorem.

Theorem 3.1. Let F be the set of all states that are invariant under local unitaries of a group Sym in the sense of relation 3.3. Furthermore, let $E : S(\mathcal{H}_A \otimes \mathcal{H}_B) \to \mathbb{R}_+ \cup \{0\}$ be an entanglement monotone that is constructed via convex roof extension. A particular set of states $\{\rho_1, ..., \rho_k\} \subset F$ is chosen so that every state $\sigma(x_1, ..., x_k) \in F$ is uniquely determined by the fidelity parameters $x_j := \mathrm{Tr}(\rho_j \sigma)$ for $j \in \{1, ..., k\}$. If E is invariant under the symmetries Sym, then one can calculate it for every state in the family in the following way:

1. Find a parametrization for all pure states that have (fixed) fidelity parameters $x_1, ..., x_k$. Denote these pure states by $|\psi_\sigma\rangle$.
2. Since the entanglement monotone is constructed via convex roof extension, it can be easily computed for pure states. Compute the function $\tilde{E}(x_1, ..., x_k) := \min_\xi E(|\psi_\sigma(x_1, ..., x_k, \xi)\rangle)$, where ξ are the parameters of $|\psi_\sigma\rangle$ that are not fidelity parameters.
3. $\tilde{E}(x_1, ..., x_k)$ is not necessarily convex compute the convexification $\tilde{E}^c(x_1, ..., x_k)$ of it.
4. The identity $\tilde{E}^c(x_1, ..., x_k) = E(\sigma(x_1, ..., x_k))$ holds.

Proof. $\underline{\mathbf{E}(\sigma(\mathbf{x_1}, ..., \mathbf{x_k})) \geq \tilde{\mathbf{E}}^{\mathbf{c}}(\mathbf{x_1}, ..., \mathbf{x_k}) :}$
For $\rho \in K$, we look at a decomposition in pure states $\rho = \sum_j p_j |\phi_j\rangle \langle\phi_j|$ that achieves the optimal value of E in the convex roof extension. In [28] the convex roof is defined with the minimum. This means that the proof of the existence of such an optimal decomposition is just the proof that in [28] the convex roof is well defined. We denote the fidelities of the state ϕ_j with $\rho_1, ..., \rho_k$ as $x_1^{(j)}, ..., x_k^{(j)}$. Then from the definitions of $\tilde{E}$ and $\tilde{E}^c$ we get

$$\begin{aligned} E(\sigma(x_1, ..., x_k)) &= \sum_j p_j E(|\phi_j\rangle \langle\phi_j|) \geq \sum_j p_j \tilde{E}(x_1^{(j)}, ..., x_k^{(j)}) \\ &\geq \sum_j p_j \tilde{E}^c(x_1^{(j)}, ..., x_k^{(j)}) \geq \tilde{E}^c(x_1, ..., x_k) \end{aligned}$$

by using the equation

$$\sum_j p_j x_i^j = x_i.$$

$\underline{\mathbf{E}(\sigma(\mathbf{x_1},...,\mathbf{x_k})) \leq \tilde{\mathbf{E}}^{\mathbf{c}}(\mathbf{x_1},...,\mathbf{x_k}) :}$
For this proof we need a small lemma.

Lemma 3.1. The entanglement monotone E is again invariant under the group of symmetries $\mathcal{G}$. For pure states $|\psi\rangle$, the entanglement monotone decreases under twirling, so that

$$E\left(\mathcal{T}_{\mathcal{G}}(|\psi\rangle\langle\psi|)\right) \leq E\left(|\psi\rangle\langle\psi|\right)$$

Proof. Let ρ be a pure state. Then the twirling integral $\mathcal{T}_{\mathcal{G}}(\rho) = \int_{\mathcal{G}} dg\ g^{-1}\rho g$, which is discussed in the appendix section 7.1.1, is a particular decomposition into pure states for $\mathcal{G} \subseteq U(\mathcal{H})$. As a set of tuples we can write $\{(dg, g^{-1}\rho g)|g \in \mathcal{G}\}$. Since in the convex roof formula we have to calculate the infimum over all decompositions we get:

$$\begin{aligned} E(\mathcal{T}_{\mathcal{G}}(\rho)) &\leq \int_{\mathcal{G}} dg\ E(g^{-1}\rho g) \\ &= \int_{\mathcal{G}} dg\ E(\rho) = E(\rho) \end{aligned}$$

□

We can write down the convexification explicitly

$$\begin{aligned} &\tilde{E}^c(x_1,...,x_k) = \inf\{\sum_i t_i \tilde{E}\left(x_1^{(i)},...,x_k^{(i)}\right)|t_i \in [0,1], \sum_i t_i = 1, \\ &\exists\sigma(x_1^{(i)},...,x_k^{(i)}) \in K = \mathcal{T}_{\mathcal{G}}(S(\mathcal{H})) : \mathrm{Tr}\Big(\sigma(x_1^{(i)},...,x_k^{(i)})\rho_r\Big) = x_r^{(i)}, \sum_i t_i x_r^{(i)} = x_r)\} \\ &= \inf\{\sum_i t_i E\left(\sigma^{(i)}\right)|t_i \in [0,1], \sum_i t_i = 1, \\ &\sigma^{(i)} \in \{|\psi\rangle\langle\psi|\,|\,|\psi\rangle \in \mathcal{H}\} : \sum_i t_i \mathcal{T}_{\mathcal{G}}\left(\sigma^{(i)}\right) = \sigma(x_1,...,x_k) \in K\} \\ &\geq \inf\{\sum_i t_i E\left(\sigma^{(i)}\right)|t_i \in [0,1], \sum_i t_i = 1, \\ &\sigma^{(i)} \in \{|\psi\rangle\langle\psi|\,|\,|\psi\rangle \in \mathcal{H}\} : \sum_i t_i \sigma^{(i)} = \sigma(x_1,...,x_k) \in K\} \\ &= E\left(\sigma(x_1,...,x_k)\right). \end{aligned}$$

The reason for the inequality is that $\sum_i t_i \mathcal{T}_{\mathcal{G}}\left(\sigma^{(i)}\right) = \sigma(x_1,...,x_k)$ is implied by $\sum_i t_i \sigma^{(i)} = \sigma(x_1,...,x_k)$ by applying the twirling operator.

□

4 Family of local cyclic permutation invariant states

In [23] a family of density matrices $\rho^{\diamondsuit}$ is introduced, which conincides with the states described above for $G = \mathbb{Z}_d$. These are studied for dimension $d = 3$. The main problem this thesis wants to address is the generalisation of $\rho^{\diamondsuit}$ to higher dimensions. One aim for this is to get insight into bound entanglement in high dimensions. In general such families of symmetric states are a good testbed for concepts in entanglement theory.

A straightforward generalisation of the density matrices $\rho^{\diamondsuit}$ to arbitrary dimension is given by

$$\begin{pmatrix}
x_1 & 0 & 0 & & & & y_{d-1} & & & & & & y_2 & & \cdots & y_1 \\
0 & x_2 & 0 & & & & & & & & & & & & & \\
0 & 0 & x_3 & & & & & & & & & & & & & \\
& & & \ddots & & & & & & & & & & & \ddots & \\
& & & & x_d & & & & & & & & & & & \\
& & & & & x_d & & & & & & & & & & \\
y_1 & & & & & & x_1 & & & & & & y_{d-1} & & & \\
& & & & & & & x_2 & & & & & & & & \\
& & & & & & & & \ddots & & & & & & \ddots & \\
& & & & & & & & & x_{d-1} & & & & & & \\
& & & & & & & & & & x_{d-1} & & & & & \\
& & & & & & & & & & & x_d & & & & \\
y_2 & & & & & & y_1 & & & & & & x_1 & & & \\
& & & & & & & & & & & & & x_2 & & \\
\vdots & & \ddots & & & & & & \ddots & & & & & & \ddots & \\
y_{d-1} & & & & & & & & & & & & & & & x_1
\end{pmatrix}.$$

This matrix still fulfills the symmetries that are imposed to $\rho^{\diamondsuit}$ in [23]:

(a) Simultaneous cyclic permutations of the basis elements of both parties, i.e. $|ij\rangle\langle kl| \mapsto |i \oplus 1\ j \oplus 1\rangle\langle k \oplus 1\ l \oplus 1|$.

(b) Simultaneous local phase rotations of the form $V(\varphi_1, \varphi_2, ..., \varphi_{d-1}) = e^{i\sum_j \varphi_j \mathfrak{g}_j} \otimes e^{-i\sum_j \varphi_j \mathfrak{g}_j}$, where $\varphi_1, ..., \varphi_{d-1}$ are real parameters and $\mathfrak{g}_j$ are the diagonal generators of SU(d).

The matrix has to be Hermitian in order to still be a density matrix. Therefore the parameters y_i need to fulfil $y_i = y_{d-i}^*$.

We want to find conditions for the parameters, so that this matrix is positive semi-definite. For this we consider the equivalent matrix

$$\begin{pmatrix}
x_1 & y_{d-1} & y_{d-2} & y_{d-3} & \cdots & y_1 & & & & & & \\
y_1 & x_1 & y_{d-1} & y_{d-2} & & & & & & & & \\
y_2 & y_1 & x_1 & y_{d-1} & \ddots & & & & & & & \\
y_3 & y_2 & y_1 & x_1 & \ddots & y_{d-2} & & & & & & \\
\vdots & & \ddots & \ddots & \ddots & y_{d-1} & & & & & & \\
y_{d-1} & & & y_2 & y_1 & x_1 & & & & & & \\
& & & & & & x_2 & & & & & \\
& & & & & & & \ddots & & & & \\
& & & & & & & & x_2 & & & \\
& & & & & & & & & x_3 & & \\
& & & & & & & & & & \ddots & \\
& & & & & & & & & & & \ddots \\
& & & & & & & & & & & & x_d
\end{pmatrix},$$

where we changed the order of the basis. One sees that the lower diagonal entries are eigenvalues. Therefore it is necessary for positivity of the matrix that for all $i \neq 1$ the parameter x_i is non negative. In the upper left corner there is a circulant matrix. Its eigenvalues are given by: $\lambda_j = x_1 + \sum_{k=1}^{d-1} \omega_j^k y_k$, where ω_j are the n-th roots of unity and can be expressed as $\omega_j = e^{\frac{2\pi i j}{d}}$. Therefore, since $\lambda_j \geq 0$ the parameters for the off-diagonal elements need to fulfil the inequality

$$\begin{aligned}
\lambda_j =& x_1 + \sum_{k=1}^{d-1} e^{\frac{2\pi i j k}{d}} y_k \\
&= x_1 + \sum_{k=1}^{\lfloor \frac{d-1}{2} \rfloor} \left(e^{\frac{2\pi i j k}{d}} y_k + e^{-\frac{2\pi i j k}{d}} y_{d-k} \right) + 2(\frac{d-1}{2} - \lfloor \frac{d-1}{2} \rfloor) y_{\lceil \frac{d-1}{2} \rceil} e^{\frac{2\pi i j}{d} \lceil \frac{d-1}{2} \rceil} \\
&= x_1 + \sum_{k=1}^{\lfloor \frac{d-1}{2} \rfloor} \left(e^{\frac{2\pi i j k}{d}} y_k + e^{-\frac{2\pi i j k}{d}} y_k^* \right) - 2(\frac{d-1}{2} - \lfloor \frac{d-1}{2} \rfloor) y_{\lceil \frac{d-1}{2} \rceil} \\
&= x_1 + \sum_{k=1}^{\lfloor \frac{d-1}{2} \rfloor} 2 \operatorname{Re}(y_k e^{\frac{2\pi i j k}{d}}) + 2(\lfloor \frac{d-1}{2} \rfloor - \frac{d-1}{2}) y_{\lceil \frac{d-1}{2} \rceil} \\
&\geq 0 \quad \forall j \in \{0, \ldots, d-1\}.
\end{aligned}$$

From these positivity conditions we can show that the physical states form a polytope. With the convention $y_0 := x_1$ we have

$$\sum_{k=0}^{d-1} e^{\frac{2\pi i j k}{d}} y_k =: \hat{y}_j \geq 0.$$

Now we can apply the reverse discrete Fourier transform

$$y_k = \frac{1}{d} \sum_{j=0}^{d-1} \hat{y}_j e^{\frac{-2\pi i j k}{d}}.$$

From these equations we can infer that there are two types of vertices. For the first type there is a $k \in \{2, ..., d\}$, so that $x_k = \frac{1}{d}$ and all the other parameters are zero. The other type has $x_1 = \frac{1}{d}$ and the other parameters in the diagonal are zero. In this latter case the off-diagonal parameters are non-zero. Their values can be calculated with the above equation, when for one $j \in \{1, ..., d-1\}$ we have $\hat{y}_j = 1$ and for $k \neq j$ we have $\hat{y}_k = 0$. One particular vertex corresponds to the maximally entangled state. There, x_1 and $\hat{y}_0$ are maximal and the other $\hat{y}_j$ are zero. To investigate the entanglement properties of the family $\rho^{\diamondsuit}$ we apply the CCNR- and the PPT-criterion.

As we have already seen the partial transpose of a matrix like $\rho^{\diamondsuit}$ is block diagonal with 2×2 blocks. The PPT criterion states that the determinant in (3.4) is for all j and k positive for separable states. PPT-states need to fulfil:
$\forall j, k \in \{1, ..., d\} \quad x_{j-k+1} \cdot x_{k-j+d+1} - |y_{j-k}|^2 \geq 0$
$\Leftrightarrow \sqrt{x_{j-k+1} \cdot x_{k-j+d+1}} \geq |y_{j-k}| \quad \forall j, k \in \{2, ..., d\} \quad j \neq k$

$$\Leftrightarrow \sqrt{x_{i+1} \cdot x_{d+1-i}} \geq |y_i| \quad \forall i \in \{1, ..., d-1\}. \tag{4.1}$$

To search for PPT entangled states, we also calculate the CCNR criterion to detect entanglement. The realigned matrix is

$$\begin{pmatrix}
x_1 & 0 & 0 & & & x_2 & & & & & & x_{d-1} & \dots & x_d \\
0 & y_1 & 0 & & & & & & & & & & & \\
0 & 0 & y_2 & & & & & & & & & & & \\
 & & & \ddots & & & & & & & & & \ddots & \\
 & & & & y_{d-1} & & & & & & & & & \\
 & & & & & y_{d-1} & & & & & & & & \\
x_d & & & & & x_1 & & & & & & x_2 & & \\
 & & & & & & y_1 & & & & & & & \\
 & & & & & & & \ddots & & & & & \ddots & \\
 & & & & & & & & y_{d-2} & & & & & \\
 & & & & & & & & & y_{d-2} & & & & \\
 & & & & & & & & & & y_{d-1} & & & \\
x_{d-1} & & & & & x_d & & & & & & x_1 & & \\
 & & & & & & & & & & & & y_1 & \\
\vdots & & \ddots & & & & & \ddots & & & & & \ddots & \\
x_2 & & & & & & & & & & & & & x_1
\end{pmatrix}.$$

To calculate its eigenvalues we consider the equivalent matrix

$$\begin{pmatrix}
x_1 & x_2 & x_3 & x_4 & \dots & x_d & & & & & & \\
x_d & x_1 & x_2 & x_3 & & & & & & & & \\
x_{d-1} & x_d & x_1 & x_2 & \ddots & & & & & & & \\
x_{d-2} & x_{d-1} & x_d & x_1 & \ddots & x_3 & & & & & & \\
\vdots & & \ddots & \ddots & \ddots & x_2 & & & & & & \\
x_2 & & & x_{d-1} & x_d & x_1 & & & & & & \\
 & & & & & & y_1 & & & & & \\
 & & & & & & & \ddots & & & & \\
 & & & & & & & & y_1 & & & \\
 & & & & & & & & & y_2 & & \\
 & & & & & & & & & & \ddots & \\
 & & & & & & & & & & & \ddots \\
 & & & & & & & & & & & & y_{d-1}
\end{pmatrix},$$

which we obtain by changing the order of the basis. The upper left block is a circulant matrix and therefore, as before, we have formulas for the eigenvalues. The sum of the absolute value of all the eigenvalues is

$$\sum_i |\eta_i| = d \sum_j |y_j| + \sum_{j=0}^{d-1} \left| \sum_{k=0}^{d-1} x_{k+1} e^{\frac{2\pi i k j}{d}} \right| \tag{4.2}$$

and the CCNR criterion states that for separable states $\sum\limits_i |\eta_i| \leq 1$. In order to obtain explicit results from equation (4.1) and (4.2) we only consider certain facets of the polytope.

4.1 Entanglement analysis for a certain facet

We will fully characterize the set of separable states in a subfamily of $\rho^{\diamond}$ corresponding to a facet of its physicality polytope. The facet of the state polytope is given by:

$$\rho^{\diamond}_{\text{facet}} := d x_1 \left|\phi\right\rangle \left\langle\phi\right| + \sum_{k=1}^{d-1} x_k \sum_{j=0}^{d-1} \left|j \quad j \oplus k\right\rangle \left\langle j \quad j \oplus k\right|. \tag{4.3}$$

The normalisation relation is still the same:

$$d \sum_{k=1}^{d} x_k = 1.$$

We want to show that in this facet all separable states are convex combinations of $\rho_k := \frac{1}{d} \sum_{j=0}^{d-1} \left|j \quad j \oplus k\right\rangle \left\langle j \quad j \oplus k\right|$ and the state ρ_{sep}, which is defined in the way that

$\forall j \in \{1,...,d\} : \frac{1}{d^2} = x_j = y_j$. To prove that ρ_{sep} is indeed separable we give a decomposition in separable states. First we define 2^d states of the following form:

$$\forall b \in \{0,1\}^d \quad |\varphi_b\rangle := \frac{1}{d}\sum_{k=0}^{d-1}(-1)^{b_k}e^{i\omega k}|k\rangle\,.$$

We consider states of the form $|\varphi_b\rangle \otimes |\varphi_b^*\rangle$ to decompose ρ_{sep} into separable states. The following calculation shows the decomposition:

$$\begin{aligned}
&\frac{1}{2\pi 2^d}\int \mathrm{d}\omega \sum_{b\in\{0,1\}^d} |\varphi_b\rangle \otimes |\varphi_b^*\rangle \langle\varphi_b| \otimes \langle\varphi_b^*| \\
&= \frac{1}{2\pi 2^d d^2}\int \mathrm{d}\omega \sum_{b\in\{0,1\}^d}\sum_{j,k,l,m} (-1)^{b_j+b_k+b_l+b_m} e^{i\omega(j-k-l+m)} |j\rangle \otimes |k\rangle \langle l| \otimes \langle m| \\
&= \frac{1}{2^d d^2}\sum_{b\in\{0,1\}^d}\sum_{j,k,l,m} (-1)^{b_j+b_k+b_l+b_m}\delta_{j-k,l-m} |j\rangle \otimes |k\rangle \langle l| \otimes \langle m| \\
&= \frac{1}{d^2}\sum_{j,k,l,m} ((\delta_{j,k}\delta_{l,m}+\delta_{j,m}\delta_{l,k})(1-\delta_{j,l})+\delta_{j,l}\delta_{k,m})\delta_{j-k,l-m} |j\rangle \otimes |k\rangle \langle l| \otimes \langle m| \\
&= \frac{1}{d^2}\sum_{j,k,l,m} (\delta_{j,k}\delta_{l,m}(1-\delta_{j,m})+\delta_{j,l}\delta_{k,m})\delta_{j-k,l-m} |j\rangle \otimes |k\rangle \langle l| \otimes \langle m| \\
&= \frac{1}{d^2}\sum_{j,k,l,m} (\delta_{j,k}\delta_{l,m}(1-\delta_{j,m})+\delta_{j,l}\delta_{k,m}) |j\rangle \otimes |k\rangle \langle l| \otimes \langle m| \\
&= \frac{1}{d^2}\sum_{j,l}\sum_{j\neq l} |jj\rangle\langle ll| + \frac{1}{d^2}\sum_{j,k} |jk\rangle\langle jk| = \rho_{\text{sep}}. \qquad (4.4)
\end{aligned}$$

To search for other separable states, we look at the CCNR criterion given in equation (4.2) for the facet

$$\sum_i |\lambda_i| = d(d-1)x_1 + \sum_{j=0}^{d-1}\left|\sum_{k=0}^{d-1} x_{k+1}e^{\frac{2\pi ikj}{d}}\right|.$$

Applying the triangle inequality yields:

$$\begin{aligned}
\sum_i |\lambda_i| &\geq d(d-1)x_1 + \left|\sum_{j=0}^{d-1}\sum_{k=0}^{d-1} x_{k+1}e^{\frac{2\pi ikj}{d}}\right| \\
&= d(d-1)x_1 + \left|dx_1 + \sum_{k=1}^{d-1} x_{k+1}\frac{1-e^{\frac{2\pi ikd}{d}}}{1-e^{\frac{2\pi ik}{d}}}\right| \\
&= d(d-1)x_1 + \left|dx_1 + \sum_{k=1}^{d-1} x_{k+1}\frac{1-1}{1-e^{\frac{2\pi ik}{d}}}\right| \\
&= d(d-1)x_1 + |dx_1| \\
&= d^2x_1.
\end{aligned}$$

Therefore we know that if $x_1 > \frac{1}{d^2}$ the state is entangled according to the CCNR-criterion, presented in section 2.2.3. By its negation, separability implies that $x_1 \leq \frac{1}{d^2}$.

We now give an example for some PPT-entangled states with

$$\begin{aligned} &x_1 \leq \frac{1}{d^2}, \quad \beta \in [0, x_1], \quad l \in \{2, ..., \lfloor \frac{d}{2} \rfloor\} \\ &\forall k \in \{2, ..., d\} \setminus \{l, d-l+2\} \\ &\quad x_k = x_1, \quad x_l = x_1 - \beta, \quad x_{d+2-l} = \frac{1}{d} - (d-1)x_1 + \beta. \end{aligned} \tag{4.5}$$

We calculate the CCNR-criterion for these states:

$$\begin{aligned} \sum |\lambda_i| &= d(d-1)x_1 + \frac{1}{d} + \sum_{j=1}^{d-1} \left| \sum_{k=0}^{d-1} x_k e^{\frac{2\pi i j k}{d}} \right| \\ &= d(d-1)x_1 + \frac{1}{d} + \sum_{j=1}^{d-1} \left| -\beta e^{\frac{2\pi i j l}{d}} + (\frac{1}{d} - dx_1 + \beta) e^{\frac{2\pi i j (d+2-l)}{d}} \right| \\ &= d(d-1)x_1 + \frac{1}{d} + \sum_{j=1}^{d-1} \left| e^{\frac{4\pi i j (1-l)}{d}} (\frac{1}{d} - dx_1 + \beta) - \beta \right| \\ &\geq d(d-1)x_1 + \frac{1}{d} + \sum_{j=1}^{d-1} \left| \left| e^{\frac{4\pi i j (1-l)}{d}} (\frac{1}{d} - dx_1 + \beta) \right| - |\beta| \right| \\ &= d(d-1)x_1 + \frac{1}{d} + (d-1)((\frac{1}{d} - dx_1 + \beta) - \beta) \\ &= d(d-1)x_1 + \frac{1}{d} + (d-1)(\frac{1}{d} - dx_1) \\ &= 1, \end{aligned}$$

where we applied the reverse triangle inequality. Since $e^{\frac{4\pi i j (1-l)}{d}}$ is not equal to 1 for all j, the inequality is not tight. Next we calculate for which values of β the states are PPT. For the states described in (4.5), Inequality (4.1) reads

$$\begin{aligned} x_1 \leq& \sqrt{(x_1 - \beta)(\frac{1}{d} - (d-1)x_1 + \beta)} \\ =& \sqrt{(\frac{1}{d} - dx_1)(x_1 - \beta) + x_1^2 - \beta^2} \\ \Leftrightarrow 0 \leq& (\frac{1}{d} - dx_1)(x_1 - \beta) - \beta^2 \\ \Leftrightarrow 0 \geq& \beta^2 + (\frac{1}{d} - dx_1)\beta - (\frac{1}{d} - dx_1)x_1. \end{aligned}$$

We check for which β the equality is fulfilled:

$$\beta_\pm = -\frac{\frac{1}{d} - dx_1}{2} \pm \sqrt{\frac{(\frac{1}{d} - dx_1)^2}{4} + (\frac{1}{d} - dx_1)x_1}.$$

for the case that there is a plus sign the solution is positive (β_+) and the state is PPT entangled for $\beta \in [0, \beta_+]$.
In this section we restricted our analysis of entanglement properties to a facet of the state polytope. We proved that the state ρ_{sep}, where all matrix elements have the same value, is separable. This helped us to find an example for PPT entangled states in our family. In the next section we want to prove that all separable states are in the polytope spanned by ρ_{sep} and the vertices that correspond to states with diagonal density matrices.

4.1.1 Separability problem

In [23] a method is described to calculate the linear entropy of states that are invariant under an entanglement preserving symmetry. It can be applied as follows. The set $\{|\phi\rangle\langle\phi|, \rho_1, ..., \rho_{d-1}\}$ consists of states that span the facet we are interested in. They are invariant under the symmetries, which were used to construct these states. One can parametrize the fidelities of some arbitrary state as follows:

$$\forall k \in \{1, ..., d-1\} \quad \mathrm{tr}(\rho\rho_k) = x_{k+1} \quad \wedge \quad \mathrm{tr}(\rho\,|\psi\rangle\langle\psi|) = dx_1.$$

A state in our facet $\sigma_{x_1,...,x_d}$ is uniquely determined by the parameters $x_1, ..., x_d$. With theorem 3.1 we can get a formula for the linear entropy. Explicitly we have to do the following steps:

1. Find a parametrization for all pure states that have the (fixed) fidelity parameters $x_1, ..., x_d$. Denote these pure states by $|\psi_\sigma\rangle$.
2. Compute the function $\tilde{E}_{\mathrm{lin}}(x_1, ..., x_d) = \min_\xi E_{\mathrm{lin}}(|\psi_\sigma(x_1, ..., x_d, \xi)\rangle)$, where ξ are the parameters of $|\psi_\sigma\rangle$ that are not fidelity parameters.
3. $\tilde{E}_{\mathrm{lin}}(x_1, ..., x_d)$ is not necessarily convex. Compute its convexification $\tilde{E}^c_{\mathrm{lin}}(x_1, ..., x_d)$.
4. The identity $\tilde{E}^c_{\mathrm{lin}}(x_1, ..., x_d) = E_{\mathrm{lin}}(\sigma_{x_1,...,x_d})$ holds.

In the following we construct a subset $\mathcal{K}$ of the facet that includes all separable states. This property would be fulfilled if the following would be true

$$\tilde{E}^c_{\mathrm{lin}}(x_1, ..., x_d) = 0 \Longrightarrow \sigma_{x_1,...,x_d} \in \mathcal{K}.$$

We know that the kernel of the convexified function $\tilde{E}^c_{\mathrm{lin}}(x_1, ..., x_d)$ is just the convexification of the kernel of the initial function $\tilde{E}_{\mathrm{lin}}(x_1, ..., x_d)$:

$$\{x_1, ..., x_d | \tilde{E}^c_{\mathrm{lin}}(x_1, ..., x_d) = 0\} = \{x_1, ..., x_d | \tilde{E}_{\mathrm{lin}}(x_1, ..., x_d) = 0\}^c. \tag{4.6}$$

For now we search a set that includes all states where $\tilde{E}_{\text{lin}}(x_1, ..., x_d) = 0$. This can be achieved by finding the states where $\tilde{E}_{\text{lin}}(x_1, ..., x_d) > 0$, and considering all other states. Pure states that build a decomposition of a state in the facet are of the form:

$$|\psi_\sigma\rangle = \sqrt{dx_1}\,|\psi\rangle + \sum_{k=1}^{d-1} \sqrt{dx_{k+1}} \sum_{j=0}^{d-1} a_{k,j}\,|j \quad j \oplus k\rangle\,, \tag{4.7}$$

where $\forall k \in \{1, ..., d-1\} \quad \sum_{j=0}^{d-1} |a_{k,j}|^2 = 1$ and $a_{j,k} \in \mathbb{C}$. Now, if ξ is a vector with all the $a_{j,k}$ as elements, then by using 3.2 we get the following formula:

$$\tilde{E}_{\text{lin}}(x_1, ..., x_d) = \min_{\xi} \sum_{jklm} |\psi_{jk}\psi_{lm} - \psi_{jm}\psi_{lk}|^2,$$

where $\psi_{lm} := |\psi(x_1, ..., x_d, \xi)\rangle_{lm}$. The minimisation over the complex phases is simple. For two complex numbers $r_1 e^{i\phi_1}$ and $r_2 e^{i\phi_2}$, the minimum of $\left|r_1 e^{i\phi_1} + r_2 e^{i\phi_2}\right|^2$ is achieved for $\phi_1 = \phi_2 + \pi$. Therefore our minimisation problem yields the same value if we assume all coefficients $a_{k,j}$ to be real. Also the optimal value for this minimisation is obtained by some ξ_{optimal} , since the function $E_{\text{lin}}(|\psi(x_1, ..., x_d, \xi)\rangle)$ is continuous (s. first definition of E_{lin} in equation (3.1)) and the space where ξ is an element of (direct sum of unit spheres in $\mathbb{R}^d$) is compact. This allows us to conclude that, for $\tilde{E}_{\text{lin}}(x_1, ..., x_d)$ to be zero, there has to exist a ξ so that

$$\begin{aligned} &\forall j, k, l, m \in \{0, ..., d-1\} \quad |\psi_{jk}\psi_{lm} - \psi_{jm}\psi_{lk}|^2 = 0 \\ \Leftrightarrow &\forall j, k, l, m \in \{0, ..., d-1\} \quad \psi_{jk}\psi_{lm} = \psi_{jm}\psi_{lk}. \end{aligned} \tag{4.8}$$

An implication of 4.8 is the following:

$$\forall m \in \{0, ..., d-1\} : \prod_{l=1}^{d} \psi_{ll} = \prod_{l=1}^{d} \psi_{l\; l\oplus m}.$$

For example, for $d = 3$, $\psi_{00}\psi_{11}\psi_{22} = \psi_{01}\psi_{10}\psi_{22} = \psi_{01}\psi_{12}\psi_{20}$. Inserting the state coefficients from equation 4.7, we obtain

$$(\sqrt{x_1})^d = \left(\sqrt{dx_{k+1}}\right)^d \prod_{j=0}^{d-1} a_{k,j} \leq (\sqrt{x_{k+1}})^d\,. \tag{4.9}$$

The inequality $\prod_{j=0}^{d-1} a_{k,j} \leq \left(\frac{1}{\sqrt{d}}\right)^d$, which was used here, will be proven in the appendix. Since squaring and taking the dth power are both monotone operations, the inequalities 4.9 cannot be true (regardless of ξ) if for some $k \in \{2, ..., d\} \quad x_1 > x_k$. But since the inequalities 4.9 are an implication of $\tilde{E}_{\text{lin}}(x_1, ..., x_d) = 0$ we get the true statement

$$\left(\tilde{E}_{\text{lin}}(x_1, ..., x_d) = 0 \quad \Rightarrow \quad \forall k \in \{2, ..., d\} \quad x_1 \leq x_k\right).$$

Therefore we know that the set of states where the coefficients have the property $\forall r \in \{2, ..., d\} \quad x_1 \leq x_r$ includes all the states with fidelity-parameters so that $\tilde{E}_{\text{lin}}(x_1, ..., x_d) =$

0. It is easy to see that the set of states with coefficients obeying $\forall k \in \{2, ..., d\} \quad x_1 \leq x_k$ coincides with the polytope spanned by $\rho_{\text{sep}}, \rho_1, ..., \rho_{d-1}$. According to equation (4.6) the convexification of this subset yields a set that includes all states where the linear entropy is zero. Since our subset is already convex, the convexification leaves it invariant. This shows that all separable states in the facet are convex combinations of $\rho_{\text{sep}}, \rho_1, ..., \rho_{d-1}$. But since we showed at the beginning that ρ_{sep} is separable the converse is also true and we know that all states in the polytope spanned by $\rho_{\text{sep}}, \rho_1, ..., \rho_{d-1}$ are separable.

4.1.2 Calculation of Areas

Since we found out in the last chapter which states are entangled or PPT-entangled, we can now ask the question, how big the volume of PPT-entangled states is. So we want to calculate what proportion of the states in the facet described in equation 4.3 are PPT-entangled and see how this scales with the dimension. We will also often talk about area instead of volume to emphasize that the facet is not full-dimensional. First we look at the ratio of separable states. The metric that our volume calculation should be based on is the Hilbert-Schmidt metric, because it is a standard measure for distance between density matrices. The following calculation shows that this metric can be related to the Euclidean metric for the parameters $x_1, ..., x_d$. We define two density matrices $X_1 = \sigma(x_1^{(1)}, x_2^{(1)}, ..., x_d^{(1)}), X_2 = \sigma(x_1^{(2)}, x_2^{(2)}, ..., x_d^{(2)})$ with $X_1 - X_2 = \sigma(\Delta x_1, \Delta x_2, ..., \Delta x_d)$ and $\Delta x_k := x_k^{(2)} - x_k^{(1)}$. For these two density matrices in our facet the Hilbert Schmidt norm has following form:

$$\begin{aligned}\sqrt{\text{Tr}((X_1 - X_2)(X_1 - X_2)^\dagger)} &= \sqrt{\text{Tr}(\sigma(\Delta x_1, \Delta x_2, ..., \Delta x_d)^2)} \\ &= \sqrt{d^2(\Delta x_1)^2 + d\sum_{j=2}^{d}(\Delta x_j)^2}.\end{aligned}$$

We can relate this last expression to the Euclidean norm with the following linear transformation:

$$dx_1 \to \xi_1 \quad k \in \{2, ..., d\} \ \sqrt{d}x_k \to \xi_k$$

Now we want to calculate the surface integral that takes the normalisation condition into account. We first need a parametrization $l(\xi_1, ..., \xi_{d-1})$ for the states in the facet using $d - 1$ parameters:

$$l(\xi_1, ..., \xi_{d-1}) = \begin{pmatrix} \xi_1 \\ \xi_2 \\ \vdots \\ \xi_{d-1} \\ \frac{1}{d} - \frac{\xi_1}{d^2} - \sum_{k=2}^{d-1} \frac{\xi_k}{d} \end{pmatrix}.$$

The surface element $d\sigma$ is given by the formula

$$\mathrm{d}\sigma = \left|\det\left(\frac{\partial l}{\partial \xi_1}\middle|...\middle|\frac{\partial l}{\partial \xi_{d-1}}\middle|n\right)\right|\mathrm{d}\xi_1\mathrm{d}\xi_2...\mathrm{d}\xi_{d-1},$$

where the vertical lines separate the columns of the matrix and n is orthogonal to all previous columns and normalized. Thus to calculate the surface element, we have to calculate the directional derivatives:

$$\frac{\partial l(\xi_1,...,\xi_{d-1})}{\partial \xi_j} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ -\frac{1}{d} \end{pmatrix} \quad \text{for } j \neq 1.$$

We notice that these derivatives do not depend on the values of $\xi_1, ..., \xi_{d-1}$. Therefore $\left|\det\left(\frac{\partial l}{\partial \xi_1}\middle|...\middle|\frac{\partial l}{\partial \xi_{d-1}}\middle|n\right)\right|$ can be factored out of the integral, and since we are only interested at certain fractions of the facet (e.g., the ratio of PPT entangled states), it is not necessary to calculate this determinant explicitly. What remains is the integration of $\xi_1, ..., \xi_{d-1}$ over all admissible values. This just yields the calculation of the volume of a simplex in dimension $d-1$. There are three types of vertices in the facet. These are: the point where $\xi_1 = 1$ and $\forall k \in \{2, ..., d\}\ \xi_{d-1} = 0$, all $d-2$ points where $\xi_j = \frac{1}{\sqrt{d}}$ and $\forall k \neq j \neq 1 x_k = 0$ and the point corresponding to $\forall k \{1, ..., d-1\} \xi_k = 0$. For the polytope of separable states only the vertex where $\xi_1 = 1$ differs. This vertex is replaced by the point with coordinates $\xi_1 = \frac{1}{d}$ and $\forall k \{2, ..., d-1\}\ \xi_k = \frac{1}{d\sqrt{d}}$.

In [25] a formula is derived to compute the volume V of a d-dimensional simplex:

$$V = \frac{1}{(d-1)!}\left|\det\left(\begin{pmatrix} v_1 & v_2 & ... & v_d \\ 1 & 1 & ... & 1 \end{pmatrix}\right)\right|,$$

where v_j are the vectors that point to the vertices. Since one vector is the zero-vector we have:

$$V = \frac{1}{(d-1)!}\left|\det\left(\begin{pmatrix} v_1 & v_2 & ... & v_{d-1} \end{pmatrix}\right)\right|.$$

For the whole facet we get the factor:

$$V_{\text{all states}} = \frac{1}{(d-1)!}\left(\frac{1}{\sqrt{d}}\right)^{d-2}.$$

For the separable states V is also easily computable, since $\begin{pmatrix} v_1 & v_2 & ... & v_{d-1} \end{pmatrix}$ is a triangular matrix and thus we only have to multiply the diagonal elements to get the determinant. We find

$$V_{\text{separable}} = \frac{1}{(d-1)!}\left(\frac{1}{\sqrt{d}}\right)^{d-2}\frac{1}{d}.$$

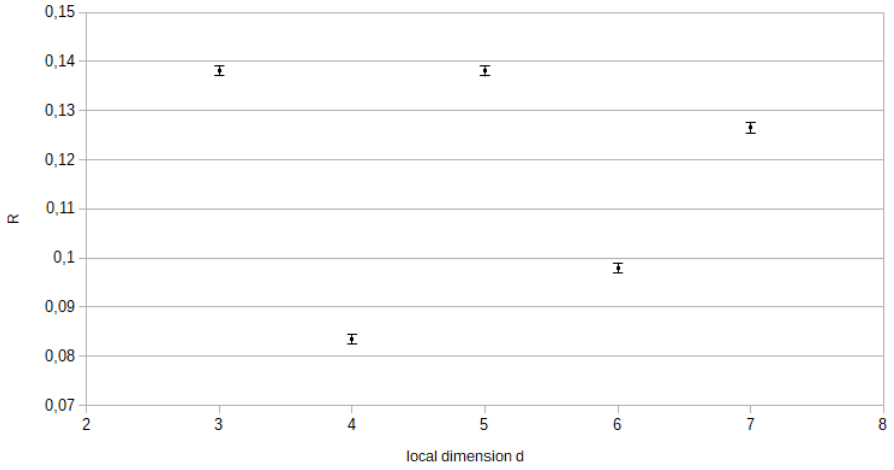

Figure 3: Ratio R between the area of the PPT-entangled states and the area of the whole facet. The results where obtained using Monte Carlo integration. The error estimation is based on section 7.2.1.

With the relation $\frac{V_{\text{separable}}}{V_{\text{all states}}} = \frac{1}{d}$ it also follows that the ratio between the area of the separable states $A_{\text{separable}}$ and the area of the whole facet obeys $A_{\text{all states}}$ the same equation:

$$\frac{A_{\text{separable}}}{A_{\text{all states}}} = \frac{1}{d}.$$

Another interesting quantity is how much area of the facet is PPT-entangled. An analytical calculation is quite difficult, since for the PPT-boundary and for the separability boundary two distinct coordinate systems would be advantageous. Instead, we have obtained some results with Monte Carlo integration, which can be seen in figure 3. The method of Monte Carlo integration is described in section 7.2.1 in the appendix.

4.1.3 Biggest Ball of PPT-Entanglement

In the previous section we were only concerned with the sheer quantity of PPT-entangled states, but for experiments the shape of the PPT-region is also important. In [24] a method is developed to find suitable quantum states for the preparation of a bound entangled state.

The usefulness of a bound entangled state for preparation is classified by how large a ball can be that has the state at its center and does only contain PPT-entangled states. For the radius r in the Hilbert-Schmidt norm the authors derived the following upper bounds using the PPT and the CCNR criterion:

$$\lambda_{\min}[\Gamma(\rho)] \geq r\sqrt{\frac{d-1}{d}} \qquad \wedge \qquad \|R(\rho)\|_1 > 1 + r\sqrt{d}. \tag{4.10}$$

Here Γ denotes the partial transpose, R denotes the realignment of the density matrix from section 2.2.3, and $\|\rho\|_1 = \mathrm{Tr}\left(\sqrt{\rho\rho^\dagger}\right)$ is the trace norm. Let us investigate the PPT condition closer. The eigenvalue equation for the partially transposed matrix is

$$\forall j,k \in \{1,...,d\}, j \neq k \quad \lambda v_{kj} = \rho_{jk,jk} v_{jk} + x_1 v_{kj}.$$

In this equation λ is the possible eigenvalue and v_{kj} are the components of the eigenvector. The indices correspond to the local systems. For $j = k$ the partial transposed matrix has only one entry on the diagonal and we see that x_1 is one of the eigenvalues. By permuting the indices j and k we get:

$$\lambda v_{jk} = \rho_{kj,kj} v_{kj} + x_1 v_{jk}.$$

For $x_1 > 0$ these two equations yield:

$$x_1 v_{jk} = (\lambda - \rho_{kj,kj})(\lambda - \rho_{jk,jk}) \frac{1}{x_1} v_{jk}.$$

If the component v_{jk} of the eigenvector is not zero the eigenvalue λ has to fulfil

$$x_1 = (\lambda - \rho_{kj,kj})(\lambda - \rho_{jk,jk}) \frac{1}{x_1}.$$

This quadratic equation can now be solved for λ. We also use that for $j < k$ we have $\rho_{jk,jk} = x_{k-j+1}$ and for $j > k \quad \rho_{jk,jk} = x_{d+1+k-j}$. The eigenvalues are of the form

$$\begin{aligned}\lambda_{1,2} &= \frac{x_{k+2} + x_{d-k}}{2} \pm \sqrt{\left(\frac{x_{k+2} + x_{d-k}}{2}\right)^2 + x_1^2 - x_{k+2} x_{d-k}} \\ &= \frac{x_{k+2} + x_{d-k}}{2} \pm \sqrt{\left(\frac{x_{k+2} - x_{d-k}}{2}\right)^2 + x_1^2}\end{aligned}$$

for $k \in \{0,...,d-2\}$.

To simplify the problem we consider states of the following form for uneven dimension d:

$$\begin{aligned}x_1 \leq \frac{1}{d^2}, \quad \forall j \in \{0,...,\lfloor \frac{d}{2} \rfloor - 2\}, \quad x_{j+2} = x_1 - \beta, \\ x_{d-j} = \frac{1 - x_1 - \frac{d-1}{2}(x_1 - \beta)}{\frac{d-1}{2}} = \frac{2}{d-1} - \frac{d+1}{d-1} x_1 + \beta.\end{aligned}$$

The smaller eigenvalue of the partial transpose is then:

$$\lambda = \frac{1}{d(d-1)} - \frac{1}{d-1} x_1 - \sqrt{(\beta + \frac{1}{d(d-1)} - \frac{d-1}{4} x_1)^2 + x_1^2}.$$

As a heuristic we try to maximize the minimum distance to the separable states in the facet, instead of the radius obtained with the CCNR-criterion in equation (4.10). Of

course this does not exclude that there could be separable states outside of the facet in close proximity. As an upper bound we calculate the distance from these states to ρ_{sep}

$$||\rho - \rho_{\text{sep}}|| = \sqrt{(d-1)d\beta^2}.$$

To be able to optimize both distances we equate them:

$$\sqrt{\frac{d}{d-1}}\lambda = \sqrt{(d-1)d\beta^2}.$$

With this equation we can eliminate β. There is now an optimal value for x_1. If we always chose this the distance scales with the dimension as can be seen in figure 4.

4.1.4 Calculation of Schmidt numbers

To get some insight into the dimensionality of entanglement of our states we want to calculate the Schmidt numbers presented in definition 2.10. In analogy to entanglement witnesses from section 2.2.1, Schmidt number witnesses play an important role in calculating Schmidt numbers. In [26] Schmidt number witnesses are introduced.

Definition 4.1. An observable W is called a Schmidt witness of class $K \in \mathbb{N}$, iff

$$\rho \in S_{K-1} \Rightarrow \operatorname{tr}(W\rho) \geq 0 \text{ and } \exists \sigma \in S_K : \operatorname{tr}(W\sigma) < 0.$$

S_K denotes the set of states that have Schmidt number equal or less than K.

Definition 4.2. A K-Schmidt witness W_1 is called finer than a K-Schmidt witness W_2 if $\{\rho \in S(\mathcal{H}) | \operatorname{Tr}(\rho W_2 < 0)\} \subset \{\rho \in S(\mathcal{H}) | \operatorname{Tr}(\rho W_1 < 0)\}$.
One calls a K-Schmidt witness optimal if there is no finer witness.

It is proven in [26] that $W = \frac{K-1}{d}\mathbb{I} - |\phi\rangle\langle\phi|$ is an optimal K-Schmidt witness. We calculate the states in the facet that are detected by this witness:

$$\begin{aligned}
\operatorname{Tr}(W\rho) &= \operatorname{Tr}\left((\frac{K-1}{d}\mathbb{I} - |\phi\rangle\langle\phi|)(a|\phi\rangle\langle\phi| + \sum_{k=1}^{d-1} b_k \sum_{j=0}^{d-1} |j \quad j\oplus k\rangle\langle j \quad j\oplus k|) \right) \\
&= \frac{K-1}{d} - \operatorname{Tr}(a|\phi\rangle\langle\phi|) \\
&= \frac{K-1}{d} - a.
\end{aligned}$$

Since we are interested in the separable states, which have Schmidt number 1, we look at the case $K = 2$. This yields

$$\begin{aligned}
&\operatorname{tr}(W\rho) \geq 0 \\
\Leftrightarrow\ &\frac{1}{d} - a \geq 0 \\
\Leftrightarrow\ &\frac{1}{d} \geq dx_1 \\
\Leftrightarrow\ &\frac{1}{d^2} \geq x_1,
\end{aligned}$$

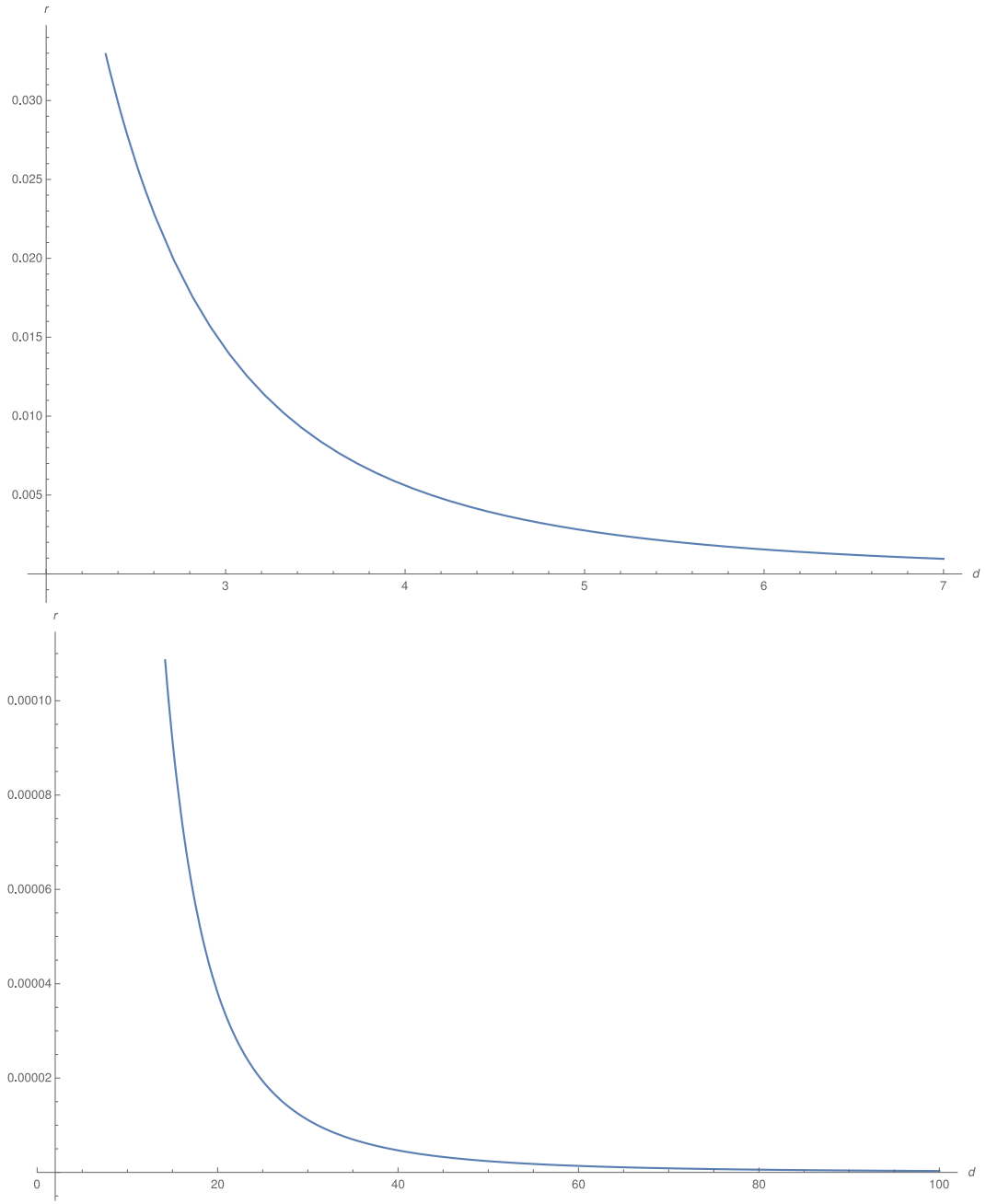

Figure 4: Upper bound on the radius r of a ball that only contains PPT-entangled states, as a function of the dimension d.

which is the same bound as the one we already derived above. Thus we try to construct another Schmidt witness that is able to detect more states with Schmidt number 2 in the facet. We know that the border between the separable states and the entangled ones is the hyperplane spanned by ρ_{sep} and the diagonal states ρ_k as defined in the beginning of section 4.1. A Schmidt witness of class 2 for dimension $d = 3$ is thus

$$W_2 = \mathbb{I} - d\,|0 \quad 1\rangle\langle 0 \quad 1| + (1-d)\,|\phi\rangle\langle\phi|\,. \tag{4.11}$$

To obtain K-Schmidt witnesses for $K > 2$ we want to move the hyperplane upwards. But the question remains how far we can displace the hyperplane so that the 3- Schmidt witness is optimal in the facet. Since the Schmidt number can be easily calculated for pure states we investigate if there are other pure states in the facet apart from $|\phi\rangle$. The purity is given by

$$\mathrm{Tr}\left(\rho^2\right) = d^2a^2 + d\sum_j b_j^2 = d(\sum_j x_j^2).$$

The state is pure iff the purity above equals 1. Since we know that the above function (parabola in multiple dimensions) is convex, we see that only $|\phi\rangle$ is a pure state.

We can achieve more insights into the Schmidt numbers of the states in the facet if we look at the full Hilbert space $\mathcal{H}\otimes\mathcal{H}$ and consider how the pure states are mapped by the twirling operator. Let $\sigma \in \mathcal{H}\otimes\mathcal{H}$ and $\mathcal{T}\sigma = \rho$. Then,

$$\begin{aligned}\forall i,j \in \{0,...,d-1\} \quad \rho_{i\ i\oplus j,i\ i\oplus j} =& \frac{1}{d}\sum_k \sigma_{k\ k\oplus j,k\ k\oplus j}\\ \rho_{i\ i,i\oplus j\ i\oplus j} =& \frac{1}{2d}\sum_k \left(\sigma_{k\ k,k\oplus j\ k\oplus j} + \sigma_{k\oplus j\ k\oplus j,k\ k}\right).\end{aligned}$$

If the twirling operator maps the state σ to the state ρ, then we know that the Schmidt number of σ is greater or equal to the Schmidt number of ρ, since twirling is a LOCC map. For simplicity we investigate the problem for dimension $d = 3$. In [23] we have the following parametrization of the pure states that are mapped in the facet by the twirling operator:

$$|\psi_\sigma\rangle = \sqrt{z}\,|\phi\rangle + \sqrt{1-z}[\sqrt{\frac{1+\overline{r}}{2}}(a\,|01\rangle + b\,|12\rangle + c\,|20\rangle) + \sqrt{\frac{1-\overline{r}}{2}}(e\,|02\rangle + f\,|10\rangle + g\,|21\rangle)].$$

Here z is a fidelity-parameter with respect to $|\phi\rangle$, $\overline{r} \in [-1,1]$ and the complex parameters a, b, c, e, f and g fulfil the normalisation conditions $|a|^2 + |b|^2 + |c|^2 = 1$ and $|e|^2 + |f|^2 + |g|^2 = 1$. For the general case it is difficult to calculate the number of non-vanishing singular values of the coefficient matrix. But if we consider states with $a = b = c$ and $e = f = g$, the coefficient matrix is circulant and one can easily calculate the eigenvalues. We get a particular easy example, if we set $\frac{1}{\sqrt{3}} = a = b = c = e = f = g$. For the case $\overline{r} = 0$ we obtain that all coefficients are equal:

$$\sqrt{\frac{z}{3}} = \sqrt{\frac{1-z}{6}} \quad \Rightarrow z = \frac{1-z}{2} \quad \Rightarrow z = \frac{1}{3}.$$

Since all entries of the coefficient matrix are equal the matrix has only one eigenvalue and therefore Schmidt number one. And indeed the state is twirled to ρ_{sep}, which was shown to be separable above. Another state we can construct has the parameters $\frac{-1}{\sqrt{3}} = a = b = c = e = f = g$. Since the coefficient matrix is circulant, one of the three eigenvalues is simply the sum over all different entries of the matrix. To get an upper bound of the Schmidt number of the state σ, we set this particular eigenvalue to zero for $\overline{r} = 0$:

$$0 = \sqrt{\frac{z}{3}} - 2\sqrt{\frac{1-z}{6}} \quad \Rightarrow z = 2(1-z) \quad \Rightarrow z = \frac{2}{3}.$$

This result is in agreement with the first Schmidt number witness W_2 in equation (4.11) that we applied, because the Schmidt witness is tangent to the state. Another state we can investigate is at $\overline{r} = 1$. We again set the same eigenvalue zero and keep in mind that the coefficients with $\sqrt{1-r}$ vanish:

$$0 = \sqrt{\frac{z}{3}} - \sqrt{2}\sqrt{\frac{1-z}{6}} \quad \Rightarrow z = (1-z) \quad \Rightarrow z = \frac{1}{2}.$$

For the $\overline{r}$-values in between we still can look at a circulant coefficient matrix and set one eigenvalue zero.

$$\begin{aligned}
&0 = \sqrt{\frac{z}{3}} - \sqrt{1-z}\left(\sqrt{\frac{1+\overline{r}}{6}} + \sqrt{\frac{1-\overline{r}}{6}}\right) \\
&\Leftrightarrow \sqrt{x_1} = \sqrt{x_2} + \sqrt{x_3} \\
&\Rightarrow x_1 = x_2 + x_3 + 2\sqrt{x_2 x_3} \\
&\Rightarrow 2x_1 = \frac{1}{3} + 2\sqrt{x_2 x_3} \\
&\Rightarrow x_1 = \frac{1}{6}\left(1 - 3x_2 \pm \sqrt{3}\sqrt{2x_2 - 9x_2^2}\right),
\end{aligned} \tag{4.12}$$

where we used the normalisation condition $x_1 + x_2 + x_3 = 1/3$.

Based on the above observations, we make the following general Ansatz for the Schmidt witness W_3:

$$W_3 = \alpha\mathbb{I} - \beta\left|\phi\right\rangle\left\langle\phi\right| - \gamma\frac{1}{3}\sum_{j=0}^{2}\left|j \quad j\oplus 1\right\rangle\left\langle j \quad j\oplus 1\right|, \quad \alpha,\beta,\gamma \in \mathbb{R}_+.$$

This is a valid Schmidt number witness if at least one state with Schmidt number 3 is detected by it and all states with Schmidt number 2 fulfil $\text{Tr}(W_3\rho) \geq 0$. The later condition is equivalent to:

$$\alpha \geq \max_{\rho \text{ has Schmidt rank } 2} \text{Tr}\left((\beta\left|\phi\right\rangle\left\langle\phi\right| + \frac{\gamma}{3}\sum_{j=0}^{2}\left|j \quad j\oplus 1\right\rangle\left\langle j \quad j\oplus 1\right|)\rho\right).$$

Note that we do not only maximize over states in the facet, since for states outside of the facet twirling could decrease the Schmidt number (or let it invariant). We now write the equal sign, because we want to detect as many states as possible. By using the linearity of the trace we get

$$\alpha = \max_{\rho \text{ has Schmidt rank } 2} \beta \operatorname{Tr}(|\phi\rangle\langle\phi|\,\rho) + \sum_{j=0}^{2} \frac{\gamma}{3} \operatorname{Tr}(|j \quad j\oplus 1\rangle\langle j \quad j\oplus 1|\,\rho).$$

We now derive an upper bound for the function we maximise over. First we look at the term $\operatorname{Tr}\Big(\sum_{j=0}^{2} |j \quad j\oplus 1\rangle\langle j \quad j\oplus 1|\,\rho\Big)$. In general we can ask, if we have diagonal matrix D with trace $\operatorname{Tr}(D) = 1$, for which density matrix ρ the term $\operatorname{Tr}(D\rho)$ is maximal. Since only the diagonal terms of ρ contribute, we can write the problem as

$$\max_{q_i} \sum_i d_i q_i \quad \text{with} \quad \sum_i q_i = 1,$$

where d_i are the diagonal terms of D and q_i the diagonal entries of ρ. The solution for this problem is that at the position i where the maximal d_i lies, q_i should be 1. For our specific problem we see that the positions of the diagonal terms of the maximal ρ should be a subset of the positions of the diagonal terms of $\sum_{j=0}^{2} |j \quad j\oplus 1\rangle\langle j \quad j\oplus 1|$.
We also use lemma 1 from [26]. It states that for any density matrix $\rho \in S(\mathbb{C}^d \otimes \mathbb{C}^d)$, which has the Schmidt number K, the following inequality is valid

$$\max_{\phi} \langle\phi|\,\rho\,|\phi\rangle \leq \frac{K}{d}, \tag{4.13}$$

where the maximisation is done over all maximally entangled states. For our purpose this lemma tells us that the fidelity with the maximally entangled state $|\phi\rangle = \frac{1}{\sqrt{3}} \sum_i |ii\rangle$ does not exceed $\frac{2}{3}$. One can argue that we only have to maximise over pure states to get the maximum, because the function we maximise over is linear in that respect. This now yields:

$$\alpha = \max_{|\eta\rangle \text{ has Schmidt rank } 2} \beta |\langle\phi|\eta\rangle|^2 + \sum_{j=0}^{2} \frac{\gamma}{3} |\langle j \quad j\oplus 1|\eta\rangle|^2.$$

The state that maximises this has to be normalized in the way that

$$|\langle\phi|\eta\rangle|^2 + \sum_{j=0}^{2} |\langle j \quad j\oplus 1|\eta\rangle|^2 = 1.$$

For the evaluation of this equation we do not use the Schmidt rank of $|\eta\rangle$ in another way than by restricting the overlap with the maximal entangled state through the inequality (4.13). Since the property that η has Schmidt rank 2 could in principle lead to a tighter restriction than the above equation alone, we again look only at an upper bound for the maximum. We thus have

$$\alpha = \max_{|\eta\rangle \text{ has Schmidt rank } 2} \beta |\langle\phi|\eta\rangle|^2 + \frac{\gamma}{3}(1 - |\langle\phi|\eta\rangle|^2).$$

Let us consider the case where $\beta \geq \frac{\gamma}{3}$. Here we know that to attain the maximum the first priority is to increase the fidelity to the maximally entangled state to $z = \frac{2}{3}$. Thus for $\beta \geq \frac{\gamma}{3}$ the witness just has to fulfil:

$$\alpha = \frac{2}{3}\beta + \frac{1}{9}\gamma.$$

For all Schmidt witnesses fulfilling this equation we can show that one with $\gamma = 0$ is the strongest. For this, we first look at states with $\overline{r} = 1$:

$$\begin{aligned}\mathrm{Tr}(W_3\rho) &= \frac{2}{3}\beta + \frac{1}{9}\gamma - bz - \gamma\frac{1-z}{3} \\ &= \frac{2}{3}\beta - \frac{2\gamma}{9} + (\frac{\gamma}{3} - \beta)z \\ &= (3\beta - \gamma)(\frac{2}{9} - \frac{z}{3}) = 0.\end{aligned}$$

This shows that these Schmidt number witnesses intersect the $\overline{r} = 1$ line at $z = \frac{2}{3}$ and for $c = 3b$ the W_3 is no witness, because no state is detected. In that case the witness coincides with the $\overline{r} = 1$-line. For $\overline{r} = 0$, we see that the most states are detected with $c = 0$. All in all, we see that the witness with $c = 0$ is finer than with other values.

The obtained results for the Schmidt numbers in the facet for dimension $d = 3$ are summarized in figure 5. For states in the yellow area we still do not know if they have Schmidt number 2 or 3. The curve between the yellow and the blue area is given by equation (4.12).

For general dimension d, we still can estimate the border between states with maximal Schmidt number and states with less than maximal Schmidt number. We start from the parametrisation of an arbitrary pure state that is twirled to the facet, which can be seen in equation (4.7). We choose $a_{k,j} = -\frac{1}{\sqrt{d}}$, so that the coefficient matrix becomes circulant. Because of this simplification, we will not find all states with maximal Schmidt number. We again set the eigenvalue that is a sum of the distinct matrix entries to zero:

$$\begin{aligned}&\sqrt{x_1} = \sum_{k=1}^{d-1}\sqrt{x_{k+1}} \\ &\Rightarrow x_1 = \left(\sum_{k=1}^{d-1}\sqrt{x_{k+1}}\right)^2 \\ &\Rightarrow x_1 = \sum_{k=1}^{d-1} x_{k+1} + \sum_{j,l=1;\ j\neq l}^{d-1}\sqrt{x_{j+1}x_{l+1}}\end{aligned}$$

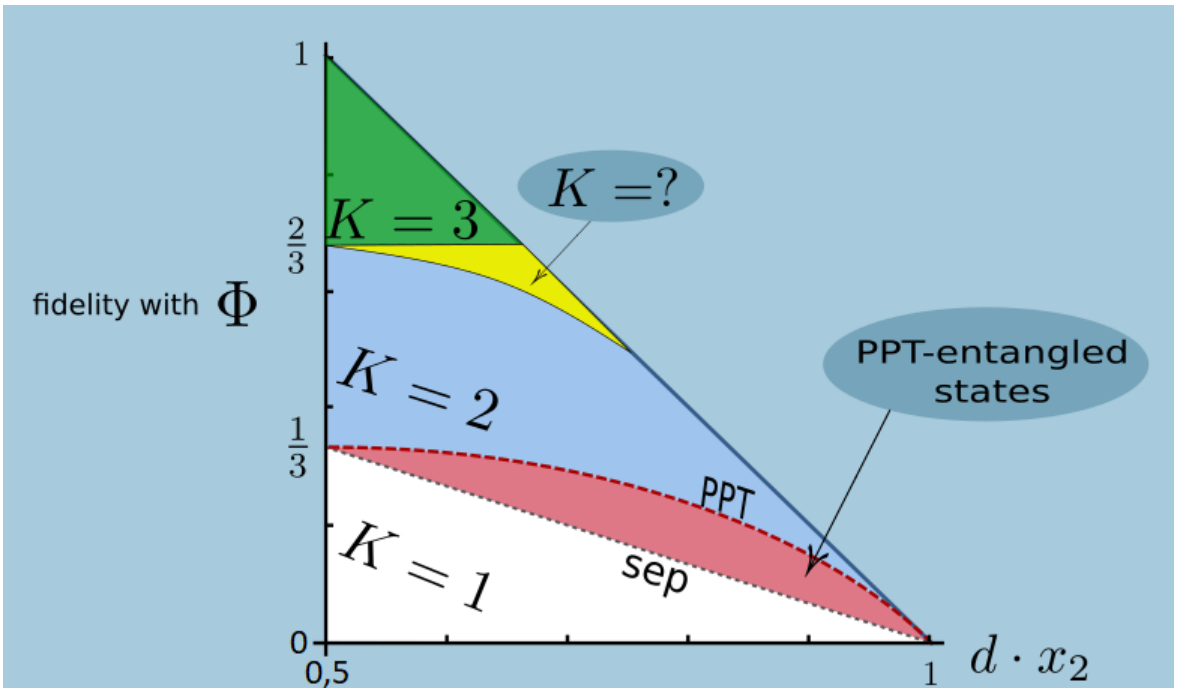

Figure 5: Progress in calculating the Schmidt numbers K of the states in the facet for $d = 3$.

With the normalisation condition $\frac{1}{d} = \sum_{k=1}^{d} x_k$ we get:

$$\Rightarrow x_1 = \frac{1}{d} - x_1 + 2\sum_{k=3}^{d}\sqrt{x_2 x_k} + \sum_{j,l=3;\ j\neq l}^{d}\sqrt{x_j x_l}$$

$$\Rightarrow 2x_1 = \frac{1}{d} + 2\sum_{k=3}^{d}\sqrt{\frac{1}{d} - x_1 - \sum_{m=3}^{d} x_m}\sqrt{x_k} + \sum_{j,l=3;\ j\neq l}^{d}\sqrt{x_j x_l}.$$

The solution of this quadratic equation is given by

$$\Rightarrow x_1 = \frac{1}{2}\cdot$$
$$\left(\frac{1}{d}\sum_{k=3}^{d} x_k \pm \left(\sum_{k=3}^{d}\sqrt{x_k}\right)\sqrt{4\left(\frac{1}{d} - \sum_{m=3}^{d} x_m\right) + \left(\sum_{m=3}^{d}\sqrt{x_m}\right)^2 - 2\left(\frac{1}{d} - \sum_{j,l=3\ j\neq l}^{d}\sqrt{x_j x_l}\right)}\right).$$

With this equation we have a lower estimate of the set of states that do not have full Schmidt rank, that goes beyond the estimate of the first, generic Schmidt-number witness from [26] that we applied.

We will now present a method, which in principle could give us an estimate for the Schmidt number regions S_K for arbitrary dimensions. The $K-$concurrence is a special entanglement monotone, which vanishes for states with Schmidt numbers smaller than K. The idea is to calculate the $K-$concurrence using the convex characteristic curve method from section 3.2. Since the 2-concurrence is the square root of the linear entropy, we see that in section 4.1.1 we actually have used the same method. However, if we want to generalise this to higher Schmidt numbers K, we will see that one cannot simply fix all complex phases in the calculation like in section 4.1.1. In [12] the $K-$concurrence is defined as

$$C_K(|\psi\rangle) = d\left(\frac{\operatorname{Tr} B^{(k)}}{\binom{d}{K}}\right)^{\frac{1}{K}}.$$

For mixed states this definition is extended with the convex roof extension. Here $B^{(K)}$ is the K-th compound matrix of $A^\dagger A$ and A is the matrix that lists all the components of $|\psi\rangle$ so that $A_{kl} := \langle kl|\psi\rangle$. The particularity of these entanglement monotones is that they vanish for states with Schmidt number less than K. We want to take advantage of this property as discussed above. Therefore we need to investigate the term $\operatorname{Tr} B^{(K)}$ closer. For the pure states in equation (4.7) we have that

$$
\begin{aligned}
\operatorname{Tr} B^{(K)} &= \sum_{i_1<\ldots<i_K} \det\Big(\big(A^\dagger A\big)_{i_1,\ldots,i_K}\Big) \\
&= \sum_{i_1<\ldots<i_K} \sum_{\sigma\in S_K} \operatorname{sgn}(\sigma) \prod_{l=1}^{K} \sum_j a^*_{ji_l} a_{ji_{\sigma(l)}} \\
&= \sum_{i_1<\ldots<i_K} \sum_{j_1,\ldots,j_K} \sum_{\sigma\in S_K} \operatorname{sgn}(\sigma) \prod_{l=1}^{K} a^*_{j_l i_l} a_{j_l i_{\sigma(l)}} \\
&= \sum_{i_1<\ldots<i_K} \sum_{j_1,\ldots,j_K} \left(\sum_{\tau\in S_K} \operatorname{sgn}(\tau) \prod_{l=1}^{K} a_{j_l i_{\tau(l)}}\right) \left(\sum_{\nu\in S_K} \operatorname{sgn}(\nu) \prod_{l=1}^{K} a^*_{j_l i_{\nu(l)}}\right) \\
&= \sum_{i_1<\ldots<i_K} \sum_{j_1,\ldots,j_K} \left|\sum_{\tau\in S_K} \operatorname{sgn}(\tau) \prod_{l=1}^{K} a_{j_l i_{\tau(l)}}\right|^2 . \qquad (4.14)
\end{aligned}
$$

In the penultimate step we used that for permutations τ, ν and $\sigma = \nu^{-1}\tau$ we have $\operatorname{sgn}(\sigma) = \operatorname{sgn}(\tau)\operatorname{sgn}(\nu)$.

For $K = 2$ the monotone is named concurrence and is simply the square root of the linear entropy. This calculation shows also why we can write the linear entropy like in equation (3.2). For the other entanglement monotones C_K it is much harder to apply the convex characteristic curve method, because the phases of the pure state $|\psi_\sigma\rangle$ from equation (4.7) would matter in the optimisation. This can be seen in equation (4.14). For $K = 2$ there are only two terms in the absolute value. If we want to minimize the whole expression one chooses the phases so that they differ by a minus sign. For $K > 2$ there are more terms in the absolute values and it is a priori not clear how to minimize the expression.

5 Additional directions of research

5.1 Exact entanglement characterization for dimension 4

5.1.1 Visualization of PPT entanglement regions

In this section we show some partial results on the entanglement characterisation of the states analysed in section 4 in the particular case of dimension $d = 4$. Fixing the dimension allows us to apply numerical methods to compute the convex characteristic curve. Furthermore with a fixed dimension it is easier to get a graphical intuition where the PPT-entangled states are located. For this we rename the state parameters $x_1, x_2, x_3, x_4, y_1, y_2$ according to the equations $x_1 = \frac{1}{16}+a$, $x_2 = \frac{1}{16}-\frac{a}{3}+e$, $x_3 = \frac{1}{16}-\frac{a}{3}+g$, $x_4 = \frac{1}{16} - \frac{a}{3} - e - g$ and $y_1 = b$, $y_2 = c$, so that we have already fulfilled the condition $\operatorname{Tr}(\rho) = 1$. The density matrix is given by:

$$\begin{pmatrix}
a+\frac{1}{16} & 0 & 0 & 0 & 0 & b & 0 & 0 \\
0 & -\frac{a}{3}+g+\frac{1}{16} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -\frac{a}{3}+e+\frac{1}{16} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -\frac{a}{3}-e-g+\frac{1}{16} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -\frac{a}{3}-e-g+\frac{1}{16} & 0 & 0 & 0 \\
b & 0 & 0 & 0 & 0 & a+\frac{1}{16} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -\frac{a}{3}+g+\frac{1}{16} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{a}{3}+e+\frac{1}{16} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
c & 0 & 0 & 0 & 0 & b & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
b & 0 & 0 & 0 & 0 & c & 0 & 0
\end{pmatrix}$$

$$\begin{pmatrix}
0 & 0 & c & 0 & 0 & 0 & 0 & b \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & b & 0 & 0 & 0 & 0 & c \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-\frac{a}{3}+e+\frac{1}{16} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -\frac{a}{3}-e-g+\frac{1}{16} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & a+\frac{1}{16} & 0 & 0 & 0 & 0 & b \\
0 & 0 & 0 & -\frac{a}{3}+g+\frac{1}{16} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -\frac{a}{3}+g+\frac{1}{16} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -\frac{a}{3}+e+\frac{1}{16} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -\frac{a}{3}-e-g+\frac{1}{16} & 0 \\
0 & 0 & b & 0 & 0 & 0 & 0 & a+\frac{1}{16}
\end{pmatrix}.$$

The eigenvalues of the 4×4 state ρ in terms of the new parameters a, b, c, g, e are:
$\{\frac{1}{16}(16a - 16c + 1), \frac{1}{16}(16a - 32b + 16c + 1), \frac{1}{16}(16a + 32b + 16c + 1), \frac{1}{48}(-16a + 48e + 3), \frac{1}{48}(-16a - 48e - 48g + 3), \frac{1}{48}(-16a + 48g + 3)\}$.

Since the positivity condition takes a simple form, we investigate states with $b = c$. Then the positivity condition reads
$-\frac{1}{16} < a < \frac{3}{16} \wedge a + 3c + \frac{1}{16} > 0 \wedge a + \frac{1}{16} > c \wedge a < 3e + \frac{3}{16} \wedge 16a + 24e < 3 \wedge a < 3g + \frac{3}{16} \wedge a + 3(e+g) < \frac{3}{16}$. These inequalities describe some higher dimensional polytope.

If we also set $e = g$ we are left with three parameters and can plot the polytope of states as can be seen in graphic 6.

We first look at the PPT criterion. The eigenvalues of the partial transposed density matrix ρ^{T_A} are
$\{\frac{1}{16}(16a + 1), \frac{1}{48}(-16a - 48c + 48e + 3), \frac{1}{48}(-16a + 48c + 48e + 3),$
$\frac{1}{48}\left(-16a - 24\sqrt{4b^2 + e^2 + 4eg + 4g^2} - 24e + 3\right),$
$\frac{1}{48}\left(-16a + 24\sqrt{4b^2 + e^2 + 4eg + 4g^2} - 24e + 3\right)\}$.

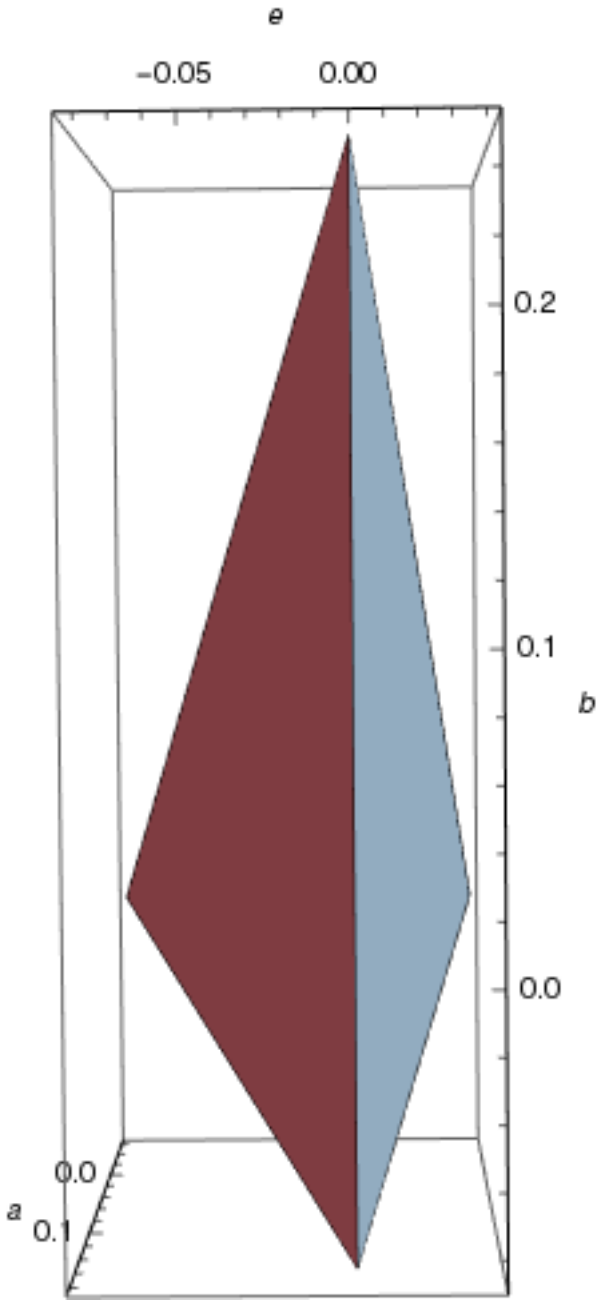

Figure 6: Tetrahedron of states with $e = g$ and $b = c$ in the space of state parameters a, b, e. The maximally entangled state sits at the vertex on top.

The PPT criterion states that the state is entangled, if one of the eigenvalues is negative. If we again set $e = g$ we can plot graphics 7 and 8, which show the positivity region together with the PPT-region.

Since we are interested in PPT entangled states we need another separability criterion. For this purpose we use the CCNR criterion. The CCNR criterion yields the inequality $\frac{2}{3}\sqrt{2}\sqrt{8a^2 - 12ae + 9e^2 + 18eg + 18g^2} + \frac{2}{3}\sqrt{(2a + 3e)^2} + 8\sqrt{b^2} + 4\sqrt{c^2} + \frac{1}{4} \geq 1$. Again, we set $g = e$ and $c = b$ and we plot the resulting CCNR-boundary in graphics 9, 10 and 11. We see that the PPT- and the CCNR-sets do not contain each other.

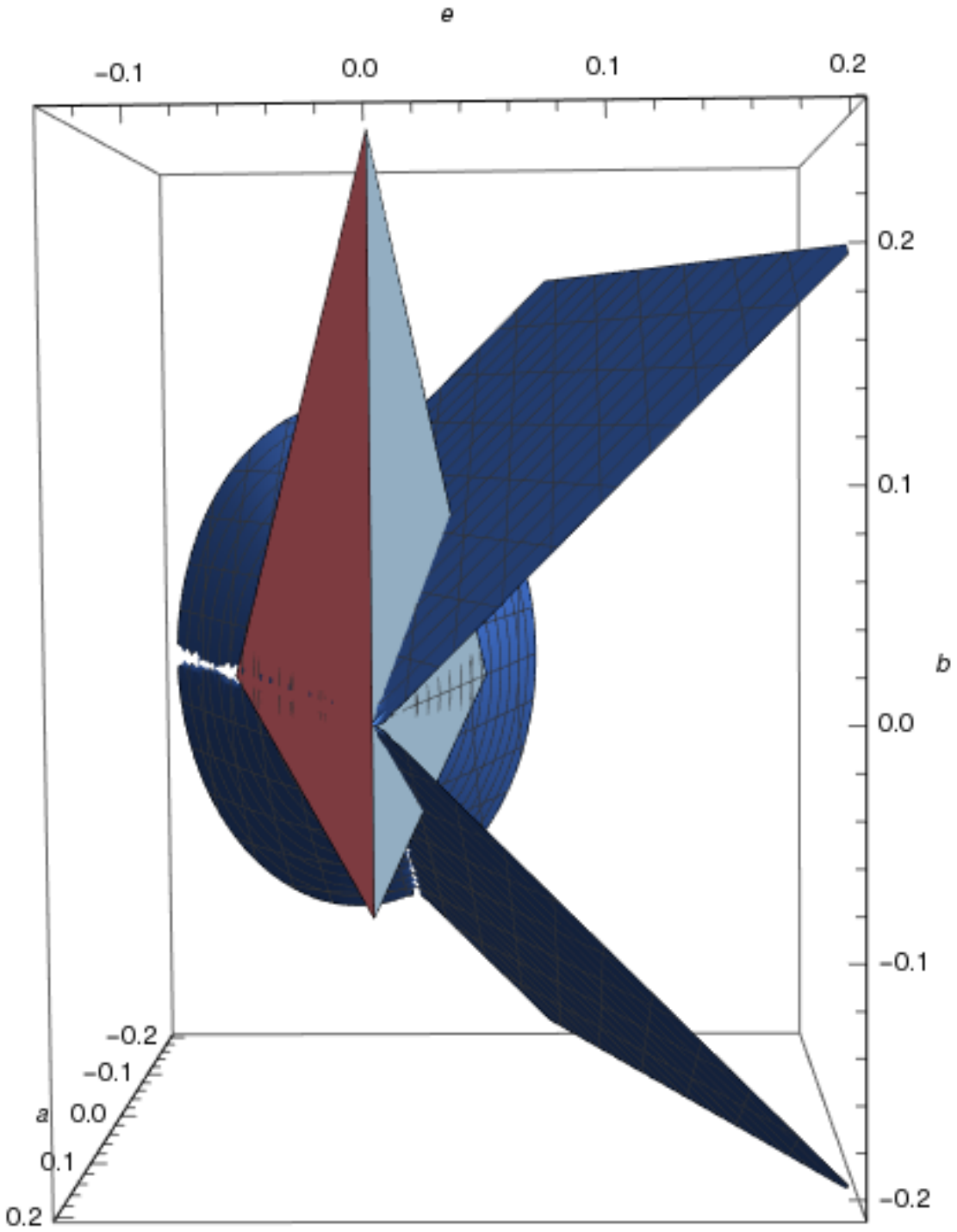

Figure 7: Tetrahedron of states together with PPT-boundary. The PPT-boundary consist of two halfplanes and a cone.

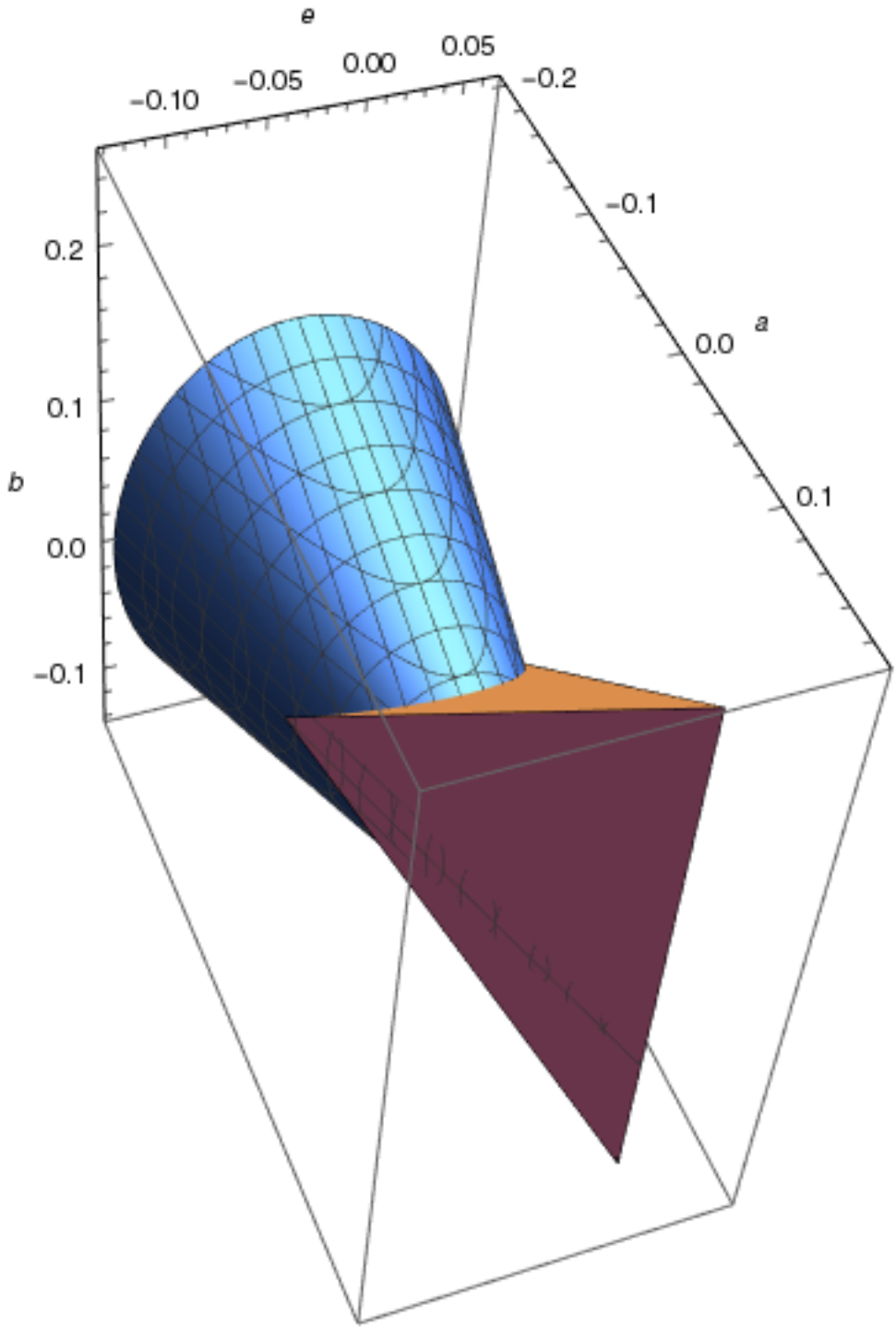

Figure 8: Tetrahedron of states together with the cone that shapes part of the PPT-boundary.

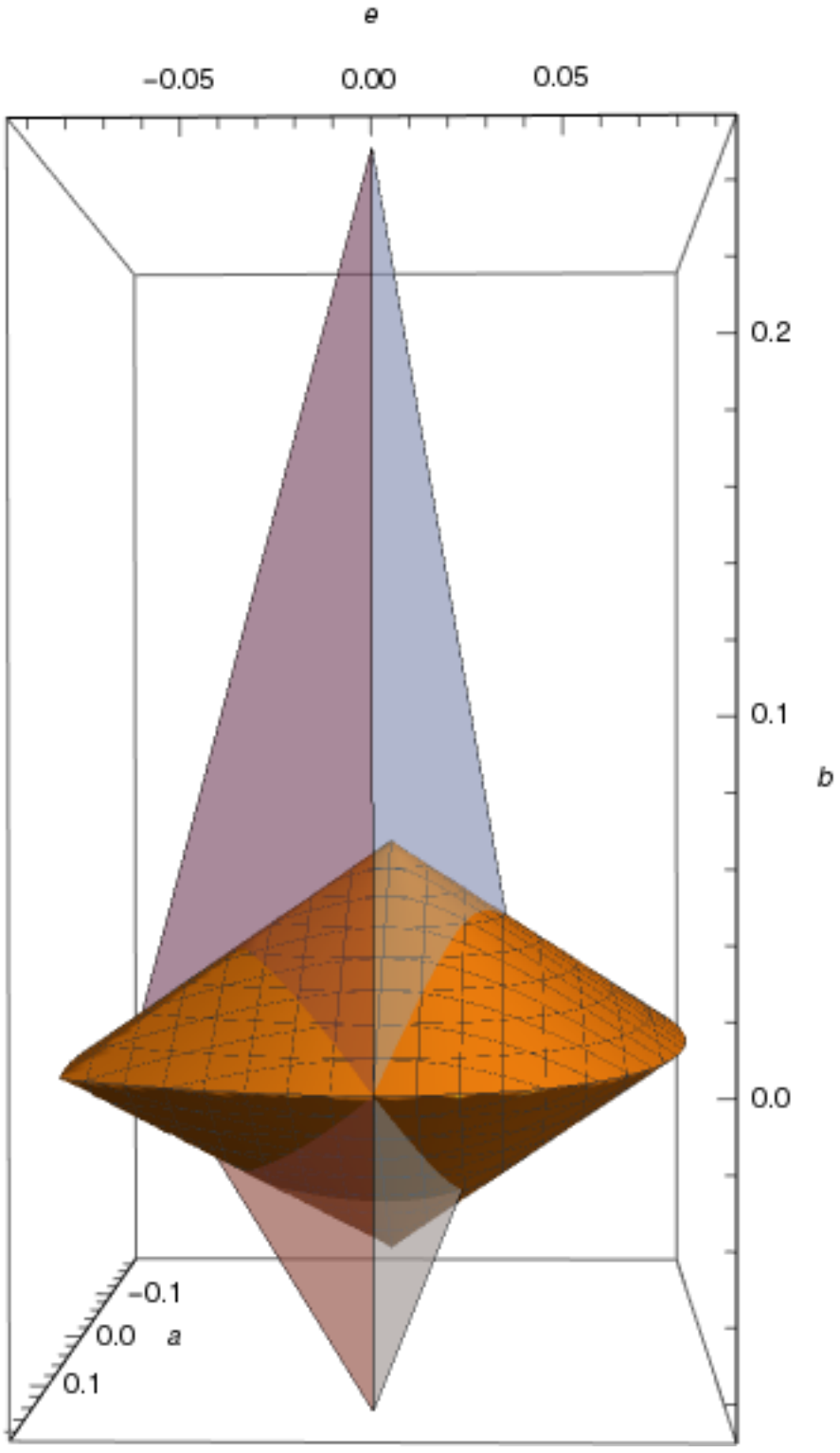

Figure 9: Tetrahedron of states together with CCNR-boundary. The CCNR-boundary is orange.

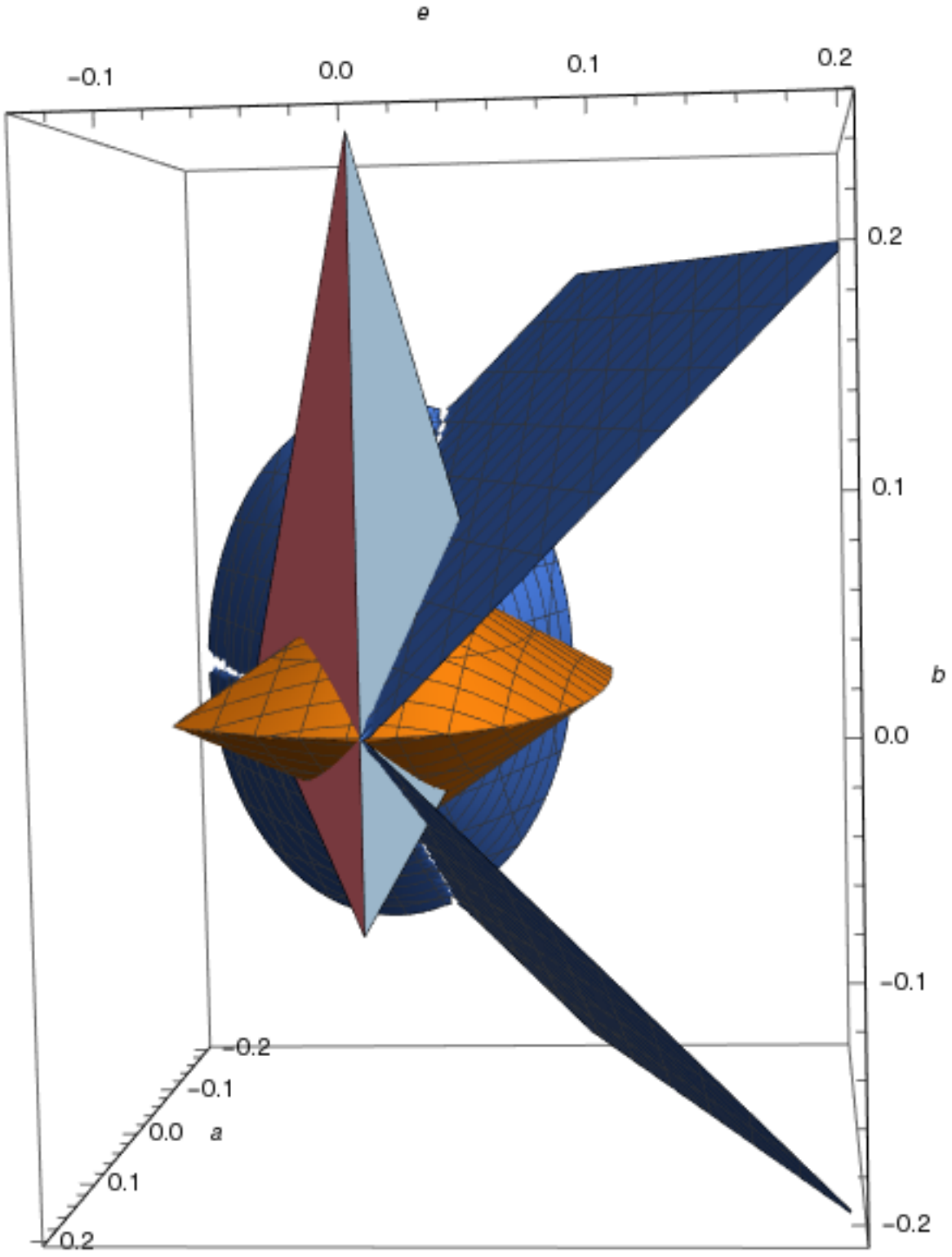

Figure 10: Tetrahedron of states together with PPT- and CCNR-boundary.

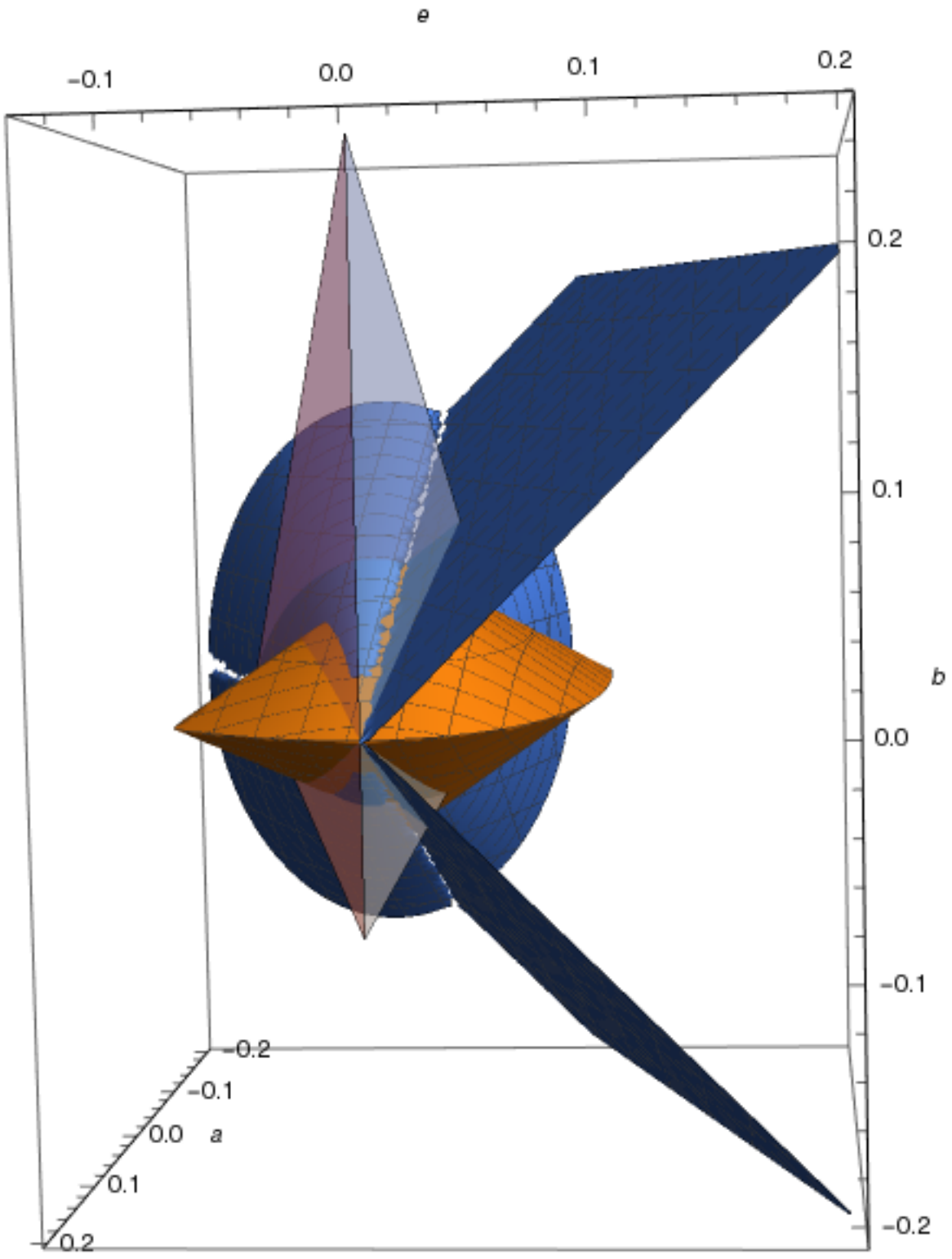

Figure 11: Tetrahedron of states together with PPT- and CCNR-boundary.

5.1.2 Computation of the linear entropy

We want to compute the convex roof extension of the linear entropy. We restrict our computation to states in the facet spanned by the points:

$$\begin{aligned}
\text{I.} \quad & a = \frac{3}{16} \quad b = \frac{1}{16} \quad e = g = 0 \\
\text{II.} \quad & a = \frac{-1}{16} \quad b = 0 \quad e = \frac{-1}{12} \quad g = \frac{1}{6} \\
\text{III.} \quad & a = \frac{-1}{16} \quad b = 0 \quad e = \frac{1}{6} \quad g = \frac{-1}{12} \\
\text{IV.} \quad & a = \frac{-1}{16} \quad b = 0 \quad e = \frac{-1}{12} \quad g = \frac{-1}{12}.
\end{aligned}$$

We will denote the states that belong to these parameters with ρ_{I}, ρ_{II}, ρ_{III} and ρ_{IV}. A state in such facet can therefore be written as

$$\sigma = z\rho_{\mathrm{I}} + (1-z)\left(y\rho_{\mathrm{II}} + (1-y)\left(x\rho_{\mathrm{III}} + (1-x)\rho_{\mathrm{IV}}\right)\right),$$

where z, y and x are parameters for the fidelities. This matrix is of rank 13. Therefore, if we look for a parametrization of the pure states in the facet, it should have $24 = 2\cdot 13 - 2$ free parameters, since the pure states of a Hilbert space H are described by the complex projective space of it. An arbitrary pure state that is twirled to the facet can be written as:

$$\begin{aligned}
|\psi_\sigma\rangle = \sqrt{z}\,|\phi\rangle + \sqrt{1-z}[\sqrt{y}\,(a\,|01\rangle + b\,|12\rangle + c\,|23\rangle + d\,|30\rangle) + \\
\sqrt{1-y}\left(\sqrt{x}\,(e\,|02\rangle + f\,|13\rangle + g\,|20\rangle + h\,|31\rangle) + \sqrt{1-x}\,(k\,|03\rangle + l\,|10\rangle + m\,|21\rangle + n\,|32\rangle)\right)],
\end{aligned} \tag{5.1}$$

where the letters from a to n without i and j in lexicographic order are complex parameters. These parameters have to fulfil:
$|a|^2 + |b|^2 + |c|^2 + |d|^2 = 1,\ |e|^2 + |f|^2 + |g|^2 + |h|^2 = 1,\ |k|^2 + |l|^2 + |m|^2 + |n|^2 = 1,\ 0 \le x \le 1,\ 0 \le y \le 1,\ 0 \le z \le 1.$

The linear entropy of a pure state is given by

$$E_{\mathrm{lin}}(\rho) = 2[(\mathrm{Tr}\,\rho_A)^2 - \mathrm{Tr}\left(\rho_A^2\right)].$$

If we have an orthonormal basis $|jk\rangle$ and a pure state ψ we can express the linear entropy as function of the state coefficients, $\psi_{jk} = \langle\psi|jk\rangle$, fulfils the equation

$$E_{\mathrm{lin}}(\psi) = \sum_{jklm} |\psi_{jk}\psi_{lm} - \psi_{jm}\psi_{lk}|^2,$$

as stated in section 3. Since for mixed states the linear entropy is defined via the convex roof method, we want to minimize the linear entropy over all these free parameters that are not x, y or z. First we look at the phases. For this we investigate one term of the sum above and use the notation $a = |a|e^{iv_a}, b = |b|e^{iv_b} ... n = |n|e^{iv_n}$. It has the form

$$\left| r_1 e^{i\phi_1} - r_2 e^{i\phi_2} \right| = r_1^2 + r_2^2 - r_1 r_2 2\cos(\phi_1 - \phi_2),$$

where $r_{1,2}$ are positive real numbers and the phases $\phi_{1,2}$ can either the phases of complex parameters like v_a or sums of to phases of the parameters $a...n$ for example $v_b + v_k$. Either way one can maximise the cosinus term and therefore minimize the whole linear entropy if one sets $v_a = v_b = v_c = v_d = v_e = v_f = v_g = v_h = v_k = v_l = v_m = v_n = 0$.

The following symmetry argument reduces the necessary parameters even more. The state coefficients from equation 5.1 can be written as the matrix

$$\begin{pmatrix} \frac{\sqrt{z}}{2} & a\sqrt{y(1-z)} & e\sqrt{x(1-y)(1-z)} & k\sqrt{(1-x)(1-y)(1-z)} \\ l\sqrt{(1-x)(1-y)(1-z)} & \frac{\sqrt{z}}{2} & b\sqrt{y(1-z)} & f\sqrt{x(1-y)(1-z)} \\ g\sqrt{x(1-y)(1-z)} & m\sqrt{(1-x)(1-y)(1-z)} & \frac{\sqrt{z}}{2} & c\sqrt{y(1-z)} \\ d\sqrt{y(1-z)} & h\sqrt{x(1-y)(1-z)} & n\sqrt{(1-x)(1-y)(1-z)} & \frac{\sqrt{z}}{2} \end{pmatrix}.$$

One notices that this matrix is invariant under simultaneous anti-transposition (flipping over the antidiagonal: $\psi_{kl} \to \psi_{(d-k)(d-l)}$ for a $d \times d$-matrix) and permutation of the parameters a and c, e and f, g and h and l and n. But since the linear entropy of $|\psi_\sigma\rangle$ is invariant under anti-transposition of the above matrix, this means that it is also invariant under simultaneous permutation of a and c, e and f, g and h and l and n.

We want to compute the minimisation

$$\min_{a,..,n} E_{\text{lin}}(|\psi_\sigma\rangle) = \min_{a,..,n} \sum_{jklm} |\psi_{jk}\psi_{lm} - \psi_{jm}\psi_{lk}|^2.$$

Purkiss principle [29] tells us that, because of the discussed symmetry, there is local extrema. Further numerical analysis indicates that one can set $a = c$, $e = f$, $g = h$ and $l = n$. Although this is a great simplification we still cannot hope to find an analytical expression for the linear entropy. Instead, we estimate the values of the linear entropy numerically for fidelities x,y and z that attain values in a $10 \times 10 \times 10$ grid. The results have then to be convexified. This method is very sensitive to numerical errors. But it nevertheless allows us to get an upper bound on the true value of the linear entropy.

To compute a lower bound on the linear entropy one can use a method from [27] based on semidefinite programming, which is discussed in the appendix. We use the Matlab programm they provide to calculate lower bounds for the same grid points in the facet. With the lower bound we can for some states definitely say that they are not entangled, because of requirement 1 in the definition of an entanglement monotone in section 3. The requirement states that a separable state is always mapped to zero.

For this grid of states, we can try to find a tight separability criterion. We try the separability criteria from [10]. This is motivated from the fact that for dimension $d = 3$

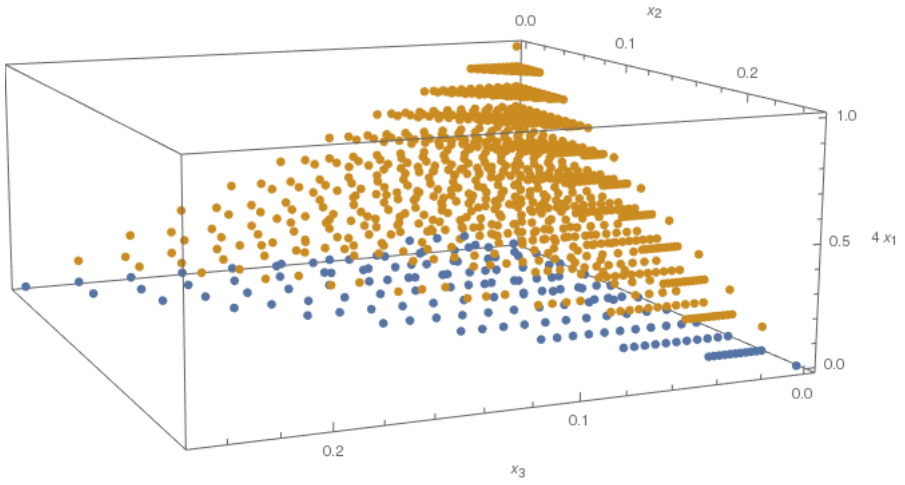

Figure 12: The orange points are shown to be entangled via the SDP-based lower bound.

in the analogous facet the CCNR-criterium is tight. As can be seen in graphics 12, 13 and 14 the CCNR criterion is not tight for dimension $d = 4$. The other separability criteria that we used detected the same states as the CCNR criterion. One of the separabilty criteria is the ZZZG-criterion from [31]. For the proof that the ZZZG criterion is stronger than the CCNR-criterion, the inequality that the geometric mean is smaller than the arithmetic mean was used as follows:

$$\sqrt{(1 - \mathrm{Tr}(\rho_A^2))(1 - \mathrm{Tr}(\rho_B^2))} \leq 1 - \frac{\mathrm{Tr}(\rho_A^2) + \mathrm{Tr}(\rho_B^2))}{2}.$$

Since for our states $\rho_A = \rho_B$, it is shown that the ZZZG criterion in this case coincides with the CCNR criterion.

5.2 Other symmetric families

In this chapter we mention other families of symmetric states. In principle these families can be analysed in the same way as the family $\rho^{\diamondsuit}$. Here in this thesis we will only describe the structure of the states and write down physicality constraints. All in all this section is more exploratory in nature.

5.2.1 Family of subsystem-permutation invariant states

Another interesting symmetry to study is the permutation of both subsystems. We want to investigate this symmetry for states which are invariant under local phase rotations like those in section 3.1. States that are invariant under local phase rotations are invariant

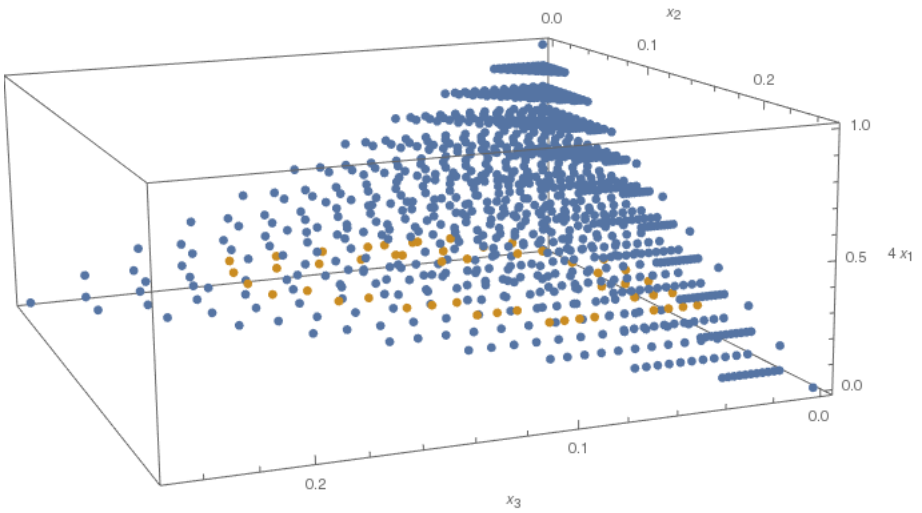

Figure 13: The orange points are shown to be entangled via the SDP-based lower bound and they are not detected by the separability criteria. The PPT-criterion is *not* used here.

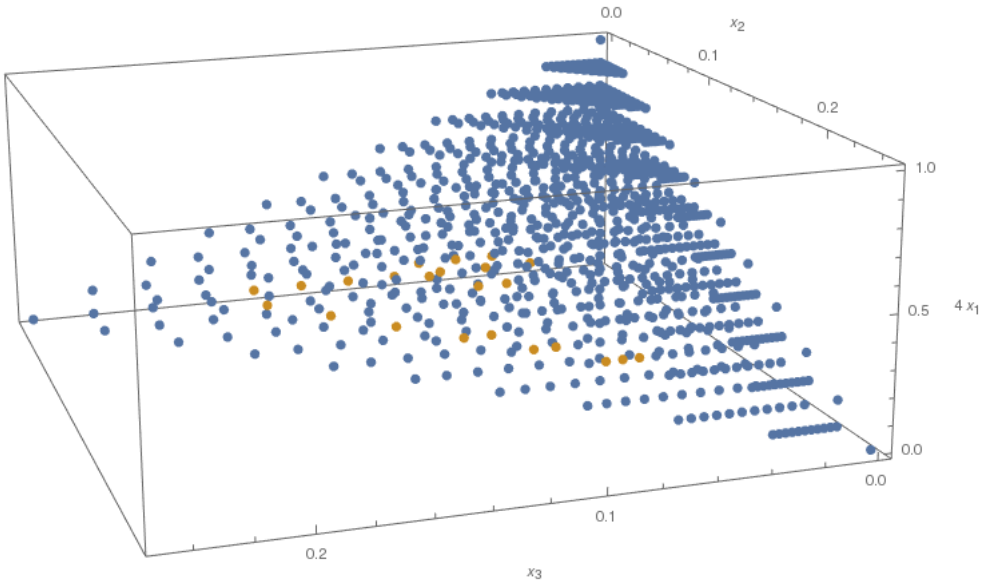

Figure 14: The orange points are shown to be entangled via the SDP-based lower bound and they are not detected by the separability criteria. Here the PPT criterium is included.

under permutation of both subsystems, fulfil:

$$\forall k, j \in \{0, ..., d-1\} \quad \rho_{jk,jk} = \rho_{kj,kj}.$$

It has to be noted that this is not a local symmetry as the ones mentioned earlier. It cannot be described as the permutation of basis vectors in the local Hilbert spaces. We want to show that there are no PPT-entangled states that fulfil both invariance constraints. To prove this we attempt to find a separable decomposition for an arbitrary PPT-state in the family.

So far we have only the following generalisation of the calculation in equation (4.4).

First we define the $2 \cdot 2^d$ states of the following form:

$$\forall b \in \{0,1\}^d \quad |\varphi_b\rangle := \sum_{k=0}^{d-1} a_k (-1)^{b_k} e^{i\omega k} |k\rangle$$
$$\forall b \in \{0,1\}^d \quad |\psi_b\rangle := \sum_{k=0}^{d-1} c_k (-1)^{b_k} e^{-i\omega k} |k\rangle .$$

where $a_k, c_k \in \mathbb{C}$ and $\sum_k |a_k|^2 = \sum_k |c_k|^2 = 1$. We always consider states of the form $|\varphi_b\rangle \otimes |\psi_b\rangle$ to decompose ρ_{sep} into separable states. The following calculation shows the decomposition:

$$\begin{aligned}
&\frac{1}{2\pi 2^d} \int \mathrm{d}\omega \sum_{b\in\{0,1\}^d} |\varphi_b\rangle \otimes |\psi_b\rangle \langle\varphi_b| \otimes \langle\psi_b| \\
&= \frac{1}{2\pi 2^d} \int \mathrm{d}\omega \sum_{b\in\{0,1\}^d} \sum_{j,k,l,m} a_j c_k a_l^* c_m^* (-1)^{b_j+b_k+b_l+b_m} e^{i\omega(j-k-l+m)} |j\rangle \otimes |k\rangle \langle l| \otimes \langle m| \\
&= \frac{1}{2^d} \sum_{b\in\{0,1\}^d} \sum_{j,k,l,m} a_j c_k a_l^* c_m^* (-1)^{b_j+b_k+b_l+b_m} \delta_{j-k,l-m} |j\rangle \otimes |k\rangle \langle l| \otimes \langle m| \\
&= \sum_{j,k,l,m} a_j c_k a_l^* c_m^* ((\delta_{j,k}\delta_{l,m} + \delta_{j,m}\delta_{l,k})(1-\delta_{j,l}) + \delta_{j,l}\delta_{k,m})\delta_{j-k,l-m} |j\rangle \otimes |k\rangle \langle l| \otimes \langle m| .
\end{aligned}$$

Since $j = m \ \wedge \ l = k \ \wedge \ j \neq k \ \wedge \ j-k = l-m$ cannot be fulfilled simultaneous we have

$$\begin{aligned}
&= \sum_{j,k,l,m} a_j c_k a_l^* c_m^* (\delta_{j,k}\delta_{l,m}(1-\delta_{j,l}) + \delta_{j,l}\delta_{k,m})\delta_{j-k,l-m} |j\rangle \otimes |k\rangle \langle l| \otimes \langle m| \\
&= \sum_{j,k,l,m} a_j c_k a_l^* c_m^* (\delta_{j,k}\delta_{l,m}(1-\delta_{j,l}) + \delta_{j,l}\delta_{k,m}) |j\rangle \otimes |k\rangle \langle l| \otimes \langle m| \\
&= \sum_{j,l \quad j\neq l} a_j c_j (a_l c_l)^* |jj\rangle \langle ll| + \sum_{j,k} |a_j|^2 |c_k|^2 |jk\rangle \langle jk| .
\end{aligned}$$

To decompose an arbitrary PPT state into separable states is still not possible, because we cannot choose the phase of every off-diagonal freely.

To describe all states in our family is obviously quite difficult, because of the positivity condition. However we can make some statements in which range of the matrix

elements the matrix cannot be positive semi-definite. Because of Sylvester's criterion it is necessary that all principal minors are not negative. In particular we have for some 2x2-minors:

$$\rho_{jj,jj}\rho_{kk,kk} \geq |\rho_{jj,kk}|^2.$$

5.2.2 Generalisation of not-completely permutation invariant qudits

In [2] another family states invariant under phase rotation (as described in section 3.1) are studied. Instead of invariance under cyclic permutations of basis elements, they allowed arbitrary permutations of the first $d-1$ basis elements. Here we generalise the idea and study states with invariance under arbitrary permutation of the first r basis vectors together with arbitrary permutations of the last $d-r$ basis elements. We restrict ourselves to real density matrices. The density matrix then depends on the real parameters a, b, c, e, f, g, h, m and n.

$$\rho_{jk,jk} = \begin{cases} a & j = k \leq r \\ b & j = k > r \\ c & j \neq k \ j \leq r \ k \leq r \\ e & j \neq k \ j \leq r \ k > r \\ f & j \neq k \ j > r \ k \leq r \\ g & j \neq k \ j > r \ k > r \end{cases} \quad \rho_{jj,kk} = \begin{cases} h & j \neq k \ j \leq r \ k \leq r \\ m & j \neq k \ j \leq r \ k > r \vee j > r \ k \leq r \\ n & j \neq k \ j > r \ k > r \end{cases}.$$

The normalisation condition $\mathrm{Tr}(\rho) = 1$ can now be formulated as

$$1 = ra + (d-r)b + r(r-1)c + r(d-r)e + (d-r)rf + (d-r)(d-r-1)g.$$

To quantify for which parameters the matrix is positive semi-definite, we use theorem 4.3 from [7]. After rearranging the density matrix the non-diagonal part can be written as $M = \begin{pmatrix} A & B \\ B^T & C \end{pmatrix}$. The diagonal elements of A are a and the off-diagonal elements are h. The diagonal elements of C are b and the off-diagonal elements are n. Every entry of B is m. We want to calculate the inverse of A and choose as Ansatz a matrix with the same structure:

$$AA^{-1} =: \begin{pmatrix} a & h & \dots & h \\ h & a & \ddots & \vdots \\ \vdots & \ddots & \ddots & \\ h & \dots & & a \end{pmatrix} \begin{pmatrix} l & p & \dots & p \\ p & l & \ddots & \vdots \\ \vdots & \ddots & \ddots & \\ p & \dots & & l \end{pmatrix} = \mathbb{I}$$
$$\Rightarrow al + (r-1)ph = 1 \quad \wedge \quad ap + lh + (r-2)ph = 0.$$

For $a \neq 0$ we get:

$$\Rightarrow l = \frac{1 - (r-1)ph}{a}.$$

We insert this in the other inequality:

$$\begin{aligned} &ap + \frac{1-(r-1)ph}{a}h + (r-2)ph = 0 \\ \Leftrightarrow &p(a - \frac{(r-1)h^2}{a} + (r-2)h) = \frac{-h}{a}. \end{aligned}$$

For $a - \frac{(r-1)h^2}{a} + (r-2)h \neq 0$ we get:

$$\Leftrightarrow p = \frac{-h}{a^2 - (r-1)h^2 + (r-2)ha}.$$

Now we can insert this again to obtain

$$l = \frac{\frac{a^2-(r-1)h^2+(r-2)ha+(r-1)h^2}{a}}{a^2 - (r-1)h^2 + (r-2)ha} = \frac{a + (r-2)h}{a^2 - (r-1)h^2 + (r-2)ha}.$$

Finally we get the inverse of the matrix A

$$A^{-1} = \frac{1}{a^2 - (r-1)h^2 + (r-2)ha} \begin{pmatrix} a+(r-2)h & -h & \dots & -h \\ -h & a+(r-2)h & \ddots & \vdots \\ \vdots & \ddots & \ddots & \\ -h & \dots & & a+(r-2)h \end{pmatrix}.$$

For $a \neq h$ we know that A has rank r and is therefore invertible. For this case the pseudo-inverse in the theorem in reference [7] is the normal inverse. The first condition that needs to be fulfilled is that A needs to be positive semi-definite. Since A is circulant we can directly calculate the eigenvalues, which need to be non-negative

$$\lambda_1 = a + (r-1)h \geq 0, \quad \lambda_2 = a - h \geq 0.$$

If A is invertible the only further condition for A to be positive semi-definite is that $D = C - B^T A^{-1} B$ has to be positive semi-definite. Moreover

$$D = \begin{pmatrix} b & n & \dots & n \\ n & b & \ddots & \vdots \\ \vdots & \ddots & \ddots & \\ n & \dots & & b \end{pmatrix} - m^2 \frac{r(a+h)}{a^2 - (r-1)h^2 + (r-2)ha} \begin{pmatrix} 1 & 1 & \dots & 1 \\ 1 & 1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \\ 1 & \dots & & 1 \end{pmatrix}.$$

All eigenvalues are non-negative if the following inequalities are fulfilled:

$$\lambda_1 = b + (d-r-1)(n - m^2 \frac{r(a+h)}{a^2 - (r-1)h^2 + (r-2)ha}) \geq 0, \quad \lambda_2 = b - n \geq 0.$$

Next we impose invariance under permutation of both subsystems. This leads to $e = f$. An interesting question is if we can still find PPT-entangled states now. In [2] they at least found no bound entangled states using the CCNR criterion. One should expect that the method we have used in this work, such as the SDP based numerical lower bound for the linear entropy, the convex characteristic curve method, and different separability criteria will shed light on the existence of PPT entanglement in this new highly symmetric family.

6 Conclusion

In this work we analysed entanglement properties of several families of symmetric states. All the families have in common that they are invariant under local phase rotations. The family we mainly looked at is additionally invariant under simultaneous local cyclic permutations of the basis elements. We showed that the state space forms a polytope. One facet of this polytope has the maximally entangled state and some diagonal density matrices ($\rho_k = \frac{1}{d}\sum_j |j\ j \oplus k\rangle\langle j\ j \oplus k|$) as vertices. For this facet we solved the separability problem with the help of the convex characteristic curve method. Since for these families of states the PPT condition are simple inequalities, we know which states are PPT-entangled. Then we calculated the ratio of the states in the facet that are separable for arbitrary dimension d. Furthermore we estimated with Monte Carlo integration the bound entangled portion of the facet for dimensions $d \leq 7$. For another estimate of the amount of bound entangled states we picked some bound entangled states in the facet and estimated what radius a ball around this state has that only contains PPT-entangled states. The result was an exponential decline in the radius of the ball at increasing local dimension d. It is still open if one can find better estimates for the exact volume of the PPT-entangled states or for the radius of the biggest ball that only contains bound entangled states. We also estimated the Schmidt numbers for the facet in dimension $d = 3$. An interesting open problem is, if there are bound entangled states with high Schmidt number in the facet. For the facet in dimension $d = 4$ we computed a SDP based lower bound of the linear entropy. We also applied several separability criteria and by comparing the results with the values for the linear entropy we showed that non of the criteria are tight.

We also presented two other families of symmetric states that are both invariant under permutation of both subsystems. In principle one could analyse these families with the same methods used in this thesis. At the moment it is not even known if they contain bound entangled states.

7 Appendix

7.1 Analytical Methods

7.1.1 Haar Measure

Results from measure theory can be applied to group theory using the Haar measure. A good introduction to the Haar measure can be found in [6].

Definition 7.1. A topological group is a group $\mathcal{G} = (G, \circ)$ equipped with a topology, so that the map of the group and the inversion of group elements are both continuous. So it is required that $G \times G \to G \quad (x, y) \mapsto x \circ y$ and $G \to G \quad g \mapsto g^{-1}$ are both continuous.

Definition 7.2. A Haar measure on a topological group $\mathcal{G}$ is a measure $\mu : \Sigma \to [0, \infty)$, where Σ is a σ-algebra that contains all Borel sets of $\mathcal{G}$, with the properties:

1. $\mu(\mathcal{G}) = 1$
2. $\forall g \in \mathcal{G}, \quad S \in \Sigma : \quad \mu(gS) = \mu(S)$

In [6] there are proofs about the existence and uniqueness of the Haar measure.

The Haar measure can be used to define an integral that attains values in a Banach-space B. One possible construction is the Bochner integral. The integral should map to $\mathcal{L}(\mathcal{H})$, which is a C^*-algebra and thus in particular a Banach-space. A starting point for defining the Bochner integral are the simple functions. They have the form:

$$s(x) = \sum_{i=1}^{n} \chi_{E_i}(x)\alpha_i,$$

where $E_i \in \Sigma$ are disjoint, $\alpha_i \in \mathcal{L}(\mathcal{H})$ and χ is the characteristic function:

$$\chi_E(x) = \begin{cases} 1 & \text{for } x \in E \\ 0 & \text{otherwise} \end{cases}.$$

For these functions the integral is defined as the sum

$$\int_{\mathcal{G}} \sum_{i=1}^{n} \chi_{E_i}(x)\alpha_i \mathrm{d}\mu = \sum_{i=1}^{n} \mu(E_i)\alpha_i.$$

With these simple functions other functions can be approximated in the sense of following definitions:

Definition 7.3. A function $f : \Sigma \to B$, where B is a Banach space, is called Bochner integrable iff it is strongly measurable and there exists a sequence of simple functions s_n so that

$$\lim_{n\to\infty} \int_{\mathcal{G}} ||f(t) - s_n(t)||_B \mathrm{d}\mu(t) = 0.$$

For Bochner integrable functions, the Bochner integral over $E \subseteq \mathcal{G}$ is defined as:

$$\int_E f \mathrm{d}\mu := \lim_{n\to\infty} \int_{\mathcal{G}} s_n \mathrm{d}\mu.$$

We will use the following theorem frequently:

Theorem 7.1. Let $L \in \mathcal{L}(B)$ be a continuous linear operator on the Banach space B. Then, if f is Bochner integrable, $L(f)$ is also Bochner integrable with

$$L\left(\int_{\mathcal{G}} f \mathrm{d}\mu\right) = \int_{\mathcal{G}} Lf \mathrm{d}\mu.$$

Using the Haar measure we can also define the twirling operator, which can be interpreted as a kind of symmetrisation. We formulate the definition from [9] directly for mixed quantum states.

Definition 7.4. Let $\mathcal{G} \subset GL(\mathcal{H})$ be a compact group that acts on $S(\mathcal{H})$ through conjugation, i.e., $\mathcal{G} \times S(\mathcal{H}) \ni (g, \rho) \mapsto g^{-1}\rho g$. The $\mathcal{G}$-Twirling operator is defined as

$$\mathcal{T}_{\mathcal{G}} : S(\mathcal{H}) \to S(\mathcal{H}) \quad \mathcal{T}_{\mathcal{G}}(\rho) = \int_{\mathcal{G}} \mathrm{d}g \; g^{-1}\rho g.$$

The integration is with respect to the Haar measure. If $\mathcal{T}_{\mathcal{G}}(\rho) = \sigma$, we can say that ρ is twirled to σ.

Definition 7.5. For fixed $\tau \in S(\mathcal{H})$ and $\rho \in S(\mathcal{H})$, we call the Hilbert-Schmidt inner product $\mathrm{Tr}\left(\tau^{\dagger}\rho\right)$ the fidelity of ρ with τ.

Lemma 7.1. If $\tau \in S(\mathcal{H})$ is invariant under the transformations $\mathcal{G}$, then for an arbitrary quantum state $\rho \in S(\mathcal{H})$ twirling does not change the fidelity with τ.

Proof.

$$\mathrm{Tr}\left(\tau \int_{\mathcal{G}} \mathrm{d}g \; g^{-1}\rho g\right) = \mathrm{Tr}\left(\int_{\mathcal{G}} \mathrm{d}g \; \tau g^{-1}\rho g\right)$$

The Hilbert space is again assumed to be finite dimensional:

$$\begin{aligned}
&= \int_{\mathcal{G}} \mathrm{d}g \;\; \mathrm{Tr}\left(\tau g^{-1}\rho g\right) \\
&= \int_{\mathcal{G}} \mathrm{d}g \;\; \mathrm{Tr}\left(g\tau g^{-1}\rho\right) \\
&= \int_{\mathcal{G}} \mathrm{d}g \;\; \mathrm{Tr}(\tau\rho) \\
&= \mathrm{Tr}(\tau\rho) \int_{\mathcal{G}} \mathrm{d}g = \mathrm{Tr}(\tau\rho)
\end{aligned}$$

□

Lemma 7.2. For $\rho \in S(\mathcal{H})$ and a compact group $\mathcal{G} \subset U(\mathcal{H})$ the following statement holds:

$$\forall U \in \mathcal{G} \quad U^{-1}\rho U = \rho \quad \Leftrightarrow \quad \exists \sigma \in S(\mathcal{H}) : \; \mathcal{T}_{\mathcal{G}}\sigma = \rho.$$

Proof. „⇒:“

$$\mathcal{T}_{\mathcal{G}}\rho = \int_{\mathcal{G}} \mathrm{d}g \; g^{-1}\rho g = \int_{\mathcal{G}} \mathrm{d}g \; \rho = \rho.$$

⇐: Since a unitary U is bounded with $||U|| = 1$, we can use Theorem 7.1 to shift the linear operators inside of the integral.

$$\begin{aligned}\forall U \in \mathcal{G} \quad U^{-1}\left(\mathcal{T}_{\mathcal{G}}\sigma\right)U &= \int_{\mathcal{G}} \mathrm{d}g \; U^{-1}g^{-1}\sigma g U \\ &= \int_{\mathcal{G}} \mathrm{d}g \; (gU)^{-1}\sigma g U \\ &= \int_{\mathcal{G}} \mathrm{d}\Big(gU^{-1}\Big) \; g^{-1}\sigma g\end{aligned}$$

Now we can make use of the invariance of the Haar measure under multiplication with a group element. (For $\mathcal{G} \subseteq GL(\mathcal{H})$ the Haar measure is invariant under multiplication of group element from right or left.)

$$\begin{aligned}\int_{\mathcal{G}} \mathrm{d}\Big(gU^{-1}\Big) \; g^{-1}\sigma g &= \int_{\mathcal{G}} \mathrm{d}(g) \; g^{-1}\sigma g \\ &= \mathcal{T}_{\mathcal{G}}\sigma.\end{aligned}$$

□

Another important fact is that if $\mathcal{G}$ has only local unitaries as elements then twirling is a LOCC operation [9].

7.1.2 Solution of the optimisation problem in section 4.1.1

In section 4.1.1 the following optimisation problem came up:

$$\max_{(a_1,\ldots,a_d)\in{\mathbb{R}_+}^d} \prod_{i=1}^{d} a_i \quad \text{under the restriction} \quad \sum_i a_i^2 = 1.$$

First we do the substitution $b_i = a_i^2$. This yields:

$$\max_{(b_1,\ldots,b_d)\in{\mathbb{R}_+}^d} \prod_{i=1}^{d} \sqrt{b_i} \quad \text{subject to} \quad \sum_i b_i = 1$$

$$\Leftrightarrow \sqrt{\max_{(b_1,\ldots,b_d)\in{\mathbb{R}_+}^d} \prod_{i=1}^{d} b_i} \quad \text{under the restriction} \quad \sum_i b_i = 1.$$

We apply the Lagrange method to find local extrema. The restricting function is $g(b_1, ..., b_d) = \sum_i b_i$. The Lagrange function is:

$$L(b_1, ..., b_d, \lambda) = \prod_{i=1}^{d} b_i + \lambda(\sum_i b_i - 1).$$

Now one has to set the gradient of this function to zero and solve the system of equations:

$$\forall k \in \{1, ..., d\} \quad \left(\prod_{i=1}^{d} b_i\right) / b_k + \lambda = 0.$$

and $\sum_i b_i = 1$. This shows that

$$\forall k \in \{1, ..., d\} \quad -\lambda = \left(\prod_{i=1}^{d} b_i\right) / b_k.$$

Which yields $b_1 = b_2 = ... = b_k = \frac{1}{d}$ and $a_1 = a_2 = ... = a_k = \frac{1}{\sqrt{d}}$. This is also a global extremum, because for boundary points one of the b_k is zero.

7.2 Computational Methods

7.2.1 Monte Carlo Integration

The idea behind Monte Carlo integration is the following. The problem is that one wants to numerically calculate a volume V that is embedded into a bigger volume Ω of known size S. Then one uniformly generates random points in the bigger volume and checks if they are contained in V. The ratio of random generated points contained in V to the total number of random generated points should optimally converge to the ratio $\frac{V}{\Omega}$. The size of the smaller volume can be expressed as the integral

$$I = \int_\Omega \chi_V(x) dx,$$

where the characteristic function is defined by $\chi_V(x) = \begin{cases} 1 & x \in V \\ 0 & \text{otherwise} \end{cases}$.
Let $x_1, ..., x_n \in \Omega$ denote the first n randomly generated points. Now we can approximate V with Q:

$$Q_n = S\frac{1}{n}\sum_{j=1}^{n} \chi_V(x_j) = S\langle\chi_V\rangle.$$

From the law of large numbers we know:

$$\lim_{n\to\infty} Q_n = I.$$

The sample variance is given by $\sigma_n^2 = \frac{1}{n-1}\sum_{j=1}^{n}(\chi_V(x_j) - Q_n)^2$ Now we get for the variance of Q_n:

$$\mathrm{Var}(Q_n) = \frac{S^2}{n^2}\sum_{j=1}^{n}\sigma_n^2 = \frac{S^2}{n}\sigma_n^2$$

If we assume that the sequence $(\sigma_n^2)_{n\in\mathbb{N}}$ is bounded, the variance of Q_n behaves asymptotically like $\frac{1}{n}$. The error of Q_n can now be estimated as follows:

$$\delta Q_n \approx \sqrt{\mathrm{Var}(Q_n)} = \frac{S}{\sqrt{n}}\sigma_n$$

The main advantage of Monte Carlo integration is that it is in principle not dependent on the dimension of the volume V.

7.2.2 Semi-definite Programming

In the field of convex optimisation semi-definite programs comprise an important class of problems. These optimisation problems are frequently encountered in quantum information theory. We will review some facts about these optimization problems from the lectures of John Watrous [30].

Definition 7.6. Let $A \in \mathcal{L}(E_1)$ and $B \in \mathcal{L}(E_2)$ be self-adjoint operators on the complex euclidean spaces E_1 and E_2. Furthermore let $\Phi : \mathcal{L}(E_1) \to \mathcal{L}(E_2)$ be a map that preserves self-adjointness. For a semi-definite program, there is a primal and a dual problem. To put it concretely, a semi-definite optimisation problem can be formulated as:

$$\begin{array}{cc} \underline{\text{primal problem}} & \underline{\text{dual problem}} \\ \text{maximize } \mathrm{Tr}(AX) & \text{minimize } \mathrm{Tr}(BY) \\ \text{subject to } \Phi(X) = B & \Phi^\dagger(Y) \geq A \\ X \geq 0 & Y \in \mathcal{L}(E_2) \end{array}$$

Before we discuss how the primal and the dual problems are related, we want to give an example.

Example 7.1. We look at primal and dual problems for the special case that $E_2 = \mathbb{C}$. Since B has to be Hermitian, it can only be represented by a matrix consisting in one real number: We have $B = 1$. For the mapping Φ, we take the trace $\Phi(X) = \mathrm{Tr}(X)$. This is a possible choice, because if X is self-adjoint the diagonal entries of the matrix are real and thus the trace is also real.

$$\begin{array}{cc} \underline{\text{primal problem}} & \underline{\text{dual problem}} \\ \text{maximize } \mathrm{Tr}(AX) & \text{minimize } \mathrm{Tr}(y) = y \\ \text{subject to } \mathrm{Tr}(X) = 1 & y\mathbb{I} \geq A \\ X \geq 0 & y \in \mathbb{R} \end{array}$$

We start by examining the primal problem. One can write the trace in the Hilbert-Schmidt scalar product with eigenvectors of A. The normalized eigenvectors of A are called $|v_j\rangle$ and their eigenvalues are λ_j. One obtains

$$\mathrm{Tr}(AX) = \sum_j \lambda_j \langle v_j | X | v_j \rangle .$$

This has to maximized under the condition $\sum_j \langle v_j | X | v_j \rangle = 1$. This is one example of a so called linear programming optimisation problem. We see that the solution is that $\mathrm{Tr}(AX)$ has to obtain the value of the highest eigenvalue of A.

Now we take a closer look at the dual problem. The following calculation shows that the dual problem as formulated above is indeed correct and the map $\mathbb{C} \ni y \mapsto y\mathbb{I} \in E_1$ is adjoint to the trace:

$$\forall X \in \mathcal{L}(E_1), y \in \mathbb{C} \quad \langle \Phi(X)|y\rangle_{\mathcal{L}(E_2)} = \mathrm{Tr}(X) \cdot y^* = \mathrm{Tr}(X(y^* \cdot \mathbb{I})) = \langle X|y\mathbb{I}\rangle_{\mathcal{L}(E_1)} .$$

We see that for the solution of the dual problem y also has to be the largest eigenvalue. Therefore for this example $\max \mathrm{Tr}(AX)$ coincides with $\min \mathrm{Tr}(BY)$ for the dual problem. In the next theorem we see that there are more problems where the dual and the primal problem have this relation.

Theorem 7.2. Slater's theorem for SDPs:
For every semi-definite program (Φ, A, B) the following statements hold:

1. Assume that there exists a positive operator X, which fulfils the constraint of the primal problem ($\Phi(X) = B$), and a self-adjoint operator Y with $\Phi^\dagger(Y) > A$. The initial constraint for the dual problem is $\Phi^\dagger(Y) \geq A$ and was therefore a weaker condition. Now the supremum in the primal problem coincides with the infimum in the dual problem and the supremum for the primal problem is attained. Supremum and infimum as mentioned here are always calculated over the operators that fulfil the restricting conditions.

2. Assume that there exists a self-adjoint operator Y, which fulfils the restricting condition of the dual problem ($\Phi^\dagger(Y) \geq A$), and a positive semi-definite operator X with $\Phi(X) = B$ and $X > 0$. Again we have in the primal problem just the condition $X \geq 0$. Now the supremum in the primal problem coincides with the infimum in the dual problem and the infimum in the dual problem is attained.

8 Symbols and Conventions

- $\mathcal{H}$: finite dimensional complex Hilbert-space
- $U(\mathcal{H})$: unitary operators on $\mathcal{H}$
- $\mathcal{L}(\mathcal{H})$: continuous endomorphisms on $\mathcal{H}$
- $\mathcal{L}_s(\mathcal{H})$: continuous self-adjoint endomorphisms on $\mathcal{H}$
- $S(\mathcal{H})$: set of states on $\mathcal{H}$.
  $S(\mathcal{H}) = \{T \in \mathcal{L}(\mathcal{H}) | \, \mathrm{tr}(T) = 1, T^\dagger = T, T \text{ is positive semi-definite})\}$
- ρ: density matrix $\rho \in S(\mathcal{H})$ for some $\mathcal{H}$
- $|0\rangle, |1\rangle, ..., |n\rangle \in \mathcal{H}$ with $n \in \mathbb{N}$: some orthonormal basis of $\mathcal{H}$

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Erklärung

Hiermit erkläre ich, dass ich die vorliegende Master-Arbeit selbstständig verfasst und keine anderen als die angegebenen Quellen und Hilfsmittel benutzt, sowie Zitate und Ergebnisse Anderer kenntlich gemacht habe.

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